

mino acid sequence for full length human wild type EPHA2 [SEQ. ID No. 1] [SEQ

<u>ID NO: 1</u>]

(Residues 596-900 are underlined)

MELQAARACFALLWGCALAAAAAAQGKEVVLLDFAAAGGELGWLTHPYGK	50
GWDLMQNIMNDMPIYMYSVCNVMSGDQDNWLRTNWVYRGEAERNNFELNF	100
TVRDCNSFPGGASSCKETFNLYYAESDLDYGTNFQKRLFTKIDTIAPDEI	150
TVSSDFEARHVKLNVEERSVGPLTRKGFYLAFQDIGACVALLSVRVYYKK	200
CPELLQGLAHFPETIAGSDAPSLATVAGTCVDHAVVPPGGEEPRMHCAVD	250
GEWLVPIGQCLCQAGYEKVEDACQACSPGFFKFEASESPCLECPEHTLPS	300
PEGATSCECEEGFFRAPQDPASMPCTRPPSAPHYLTAVGMGAKVELRWTP	350
PQDSGGREDIVYSVTCEQCWPESGECGPCEASVRYSEPPHGLTRTSVTVS	400
DLEPHMNYTFTVEARNGVSGLVTSRSFRTASVSINQTEPPKVRLEGRSTT	450
SLSVSWSIPPPQQSRVWKYEVTYRKKGDSNSYNVRRTEGFSVTLDDLAPD	500
TTYLVQVQALTQEGQGAGSKVHEFQTLSPEGSGNLAVIGGVAVGVVLLLV	550
LAGVGFF1HRRRKNQRARQSPEDVYFSKSEQLKPLKTYVDPHTYE <u>DPNQA</u>	600
VLKFTTEIHPSCVTRQKVIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKA	650
GYTEKQRVDFLGEAGIMGQFSHHNIIRLEGVISKYKPMMIITEYMENGAL	700
DKFLREKDGEFSVLQLVGMLRGIAAGMKYLANMNYVHRDLAARNILVNSN	750
LVCKVSDFGLSRVLEDDPEATYTTSGGKIPIRWTAPEAISYRKFTSASDV	800
WSFGIVMWEVMTYGERPYWELSNHEVMKAINDGFRLPTPMDCPSAIYQLM	850
MQCWQQERARRPKFADIVSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	900
SEGVPFRTVSEWLESIKMQQYTEHFMAAGYTAIEKVVQMTNDDIKRIGVR	950
LPGHQKRIAYSLLGLKDQVNTVGIPI	976

FIGURE 1A (Cont.)

Human cDNA sequence encoding residues 596-900 of EPHA2 [SEQ. ID No. 2] [SEQ ID NO: 2]

GACCCCAACCAGGCTGTTTGAAGTTCACTACCGAGATCCATCC	50
TGTCACTCGGCAGAAGGTGATCGGAGCAGGAGAGTTTGGGGAGGTGTACA	100
AGGGCATGCTGAAGACATCCTCGGGGAAGAAGGAGGTGCCGGTGGCCATC	150
AAGACGCTGAAAGCCGGCTACACAGAGAAGCAGCGAGTGGACTTCCTCGG	200
CGAGGCCGGCATCATGGGCCAGTTCAGCCACCACAACATCATCCGCCTAG	250
AGGGCGTCATCTCCAAATACAAGCCCATGATGATCATCACTGAGTACATG	300
GAGAATGGGGCCCTGGACAAGTTCCTTCGGGAGAAGGATGGCGAGTTCAG	350
CGTGCTGCAGCTGGGGCATGCTGCGGGGCATCGCAGCTGGCATGAAGT	400
ACCTGGCCAACATGAACTATGTGCACCGTGACCTGGCTGCCCGCAACATC	450
CTCGTCAACAGCAACCTGGTCTGCAAGGTGTCTGACTTTGGCCTGTCCCG	500
CGTGCTGGAGGACCCCGAGGCCACCTACACCACCAGTGGCGGCAAGA	550
TCCCCATCCGCTGGACCGCCCCGGAGGCCATTTCCTACCGGAAGTTCACC	600
TCTGCCAGCGACGTGTGGAGCTTTGGCATTGTCATGTGGGAGGTGATGAC	650
CTATGGCGAGCGGCCCTACTGGGAGTTGTCCAACCACGAGGTGATGAAAG	700
CCATCAATGATGGCTTCCGGCTCCCCACACCCATGGACTGCCCCTCCGCC	750
ATCTACCAGCTCATGATGCAGTGCTGGCAGCAGGAGCGTGCCCGCCC	800
CAAGTTCGCTGACATCGTCAGCATCCTGGACAAGCTCATTCGTGCCCCTG	850
ACTCCCTCAAGACCCTGGCTGACTTTGACCCCCGCGTGTCTATCCGGCTC	900
CCCAGCACGAGCGGC	915

Amino acid sequence for residues 596-900 of EPHA2 with a cleavable (rTev) N-terminal 6x-histidine tag [SEQ. ID No. 3] [SEQ ID NO: 3] (6x-histidine tag and cleavage site are underlined)

MSYYHHHHHHDYDIPTTENLYFQGAMGSDPNQAVLKFTTEIHPSCVTRQK	50
VIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKAGYTEKQRVDFLGEAGIM	100
GQFSHHNIIRLEGVISKYKPMMIITEYMENGALDKFLREKDGEFSVLQLV	150
GMLRGIAAGMKYLANMNYVHRDLAARNILVNSNLVCKVSDFGLSRVLEDD	200
PEATYTTSGGKIPIRWTAPEAISYRKFTSASDVWSFGIVMWEVMTYGERP	250
YWELSNHEVMKAINDGFRLPTPMDCPSAIYQLMMQCWQQERARRPKFADI	. 300
VSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	333

FIGURE 3A

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number' (SEQ ID NO: 1), (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	В	С	D	E	F		G	Н	I	J
1	N	ΔΙΔ	Δ	605	47.2	39 45	.529	67.448	1.00	51.83
2	CA			605	46.9		.860	66.049	1.00	
3	СВ			605	45.7		.876	65.490		51.40
4	C			605	46.4		.259	66.307	1.00	
5	Ō			605	46.2		.630	67.422	1.00	
6	N			606	46.2		.048	65.302	1.00	
7	CA	THR	Α	606	45.7	19 49	.337	65.564	1.00	49.98
8	СВ	THR	Α	606	46.1	28 50	.120	64.454	1.00	48.98
9	OG1	THR	Α	606	47.5	53 50	.041	64.401	1.00	50.88
10	CG2	THR	Α	606	45.7	66 51	541	64.651	1.00	48.25
11	С	THR	Α	606	44.2	01 49	.397	65.650	1.00	50.57
12	0	THR	Α	606	43.4	87 48	.868	64.787	1.00	51.60
13	N	GLU	Α	607	43.6	80 50	.086	66.646	1.00	49.68
14	CA	GLU	Α	607	42.2	64 50	.182	66.717	1.00	47.97
15	CB	GLU	Α	607	41.7	96 50	.123	68.130	1.00	47.41
16	CG	GLU	Α	607	40.3	23 50	.414	68.279	1.00	50.07
17	CD	GLU	Α	607	39.3	94 49	.230	68.074	1.00	39.82
18	OE1	GLU	Α	607	39.7	96 48	.072	68.195	1.00	38.52
19	OE2	GLU	Α	607	38.2	60 49	.515	67.856	1.00	41.61
20	C .			607	41.8		347	65.971		48.16
21	0			607	42.3		.398	66.162	1.00	
22	N			608	40.9		146	64.963	1.00	
23	CA			608	40.5		.309	64.228	1.00	
24	СВ			608	41.1		.517	62.742	1.00	
25	CG1			608	40.0		.886	61.752		49.45
26	CD1			608	39.2		.726	61.615	1.00	
27	CG2			608	42.1		.494	62.300	1.00	47.67
28	C			608	39.1		.787	64.481	1.00	51.43
29	0	ILE			38.2		.049	64.879	1.00	51.22
30 31	N CA	HIS		609	38.9 37.7		.090 .745	64.361 64.674	1.00	53.40 55.30
32	CB	HIS			37.7		5.203	65.196	1.00	57.26
33	CG	HIS			36.7		5.776	65.835	1.00	
34	ND1			609	36.4		.686	67.186	1.00	
35	CE1				35.3		.221	67.471	1.00	62.48
36	NE2	HIS			34.7		.635	66.348	1.00	63.53
37	CD2	HIS			35.6		.345	65.301	1.00	62.09
38	C	HIS			36.7		.718	63.557	1.00	53.34
39	ō			609	36.9		.109	62.474	1.00	
40	N	PRO			35.5		.263	63.854	1.00	52.90
41	CA	PRO			34.5		.113	62.805	1.00	53.20
42	СВ	PRO			33.2		.864	63.591	1.00	52.67
43	CG	PRO			33.7		.087	64.713	1.00	

FIGURE 3A (Cont.)

A	В	С	D	E	F	G	Н	I.	J
44	CD	PRO	Α	610	35.069	53.682	65.133	1.00	52.08
45	С	PRO	Α	610	34.421	55.273	61.903	1.00	52.69
46	0	PRO	Α	610	33.935	55.146	60.793	1.00	55.21
47	N	SER	Α	611	34.789	56.418	62.391	1.00	52.17
48	CA	SER	Α	611	34.546	57.584	61.639	1.00	52.33
49	CB	SER	Α	611	34.694	58.833	62.562	1.00	54.93
50	OG	SER	Α	611	35.822	58.723	63.443	1.00	49.81
51	C	SER	Α	611	35.579	57.611	60.552	1.00	52.77
52	0	SER	A	611	35.394	58.256	59.545	1.00	54.01
53	N	CYS	Α	612	36.679	56.915	60.701	1.00	49.87
54	CA	CYS	Α	612	37.633	57.083	59.642	1.00	51.06
55	CB	CYS	Α	612	39.044	56.889	60.169	1.00	50.65
56	SG	CYS	Α	612	39.193	57.805	61.702	1.00	55.75
57	С	CYS	Α	612	37.445	56.214	58.426	1.00	49.07
58	0	CYS	Α	612	38.215	56.286	57.479	1.00	48.12
59	N	VAL	Α	613	36.470	55.349	58.497	1.00	49.20
60	CA	VAL			36.329	54.361	57.471	1.00	48.42
61	CB	VAL	Α	613	36.130	52.976	58.087		49.58
62	CG1	VAL	Α	613	35.493	52.026	57.030	1.00	46.32
63	CG2	VAL	Α	613	37.477	52.423	58.651	1.00	46.61
64	С	VAL	Α	613	35.039	54.652	56.779	1.00	47.49
65	0	VAL	Α	613	34.080	55.078	57.401		46.54
66	N	THR	Α	614	34.976	54.426	55.496	1.00	46.87
67	CA	THR	Α	614	33.674	54.449	54.961	1.00	47.76
68	CB	THR	Α	614	33.230	55.839	54.547		48.10
69	OG1	THR	Α	614	32.501	55.759	53.312	1.00	53.74
70	CG2	THR	Α	614	34.430	56.804	54.383	1.00	48.56
71	С	THR	Α	614	33.479	53.362	53.956		47.36
72	0	THR	Α	614	34.145	53.317	52.971	1.00	49.44
73	N	ARG	Α	615	32.519	52.496	54.192	1.00	46.37
74	CA	ARG	Α	615	32.356	51.360	53.352	1.00	44.80
75	CB	ARG	Α	615	31.323	50.464	53.993	1.00	43.89
76	CG	ARG	Α	615	31.817	49.366	54.921	1.00	44.82
77	CD	ARG	Α	615	30.699	48.434	55.297	1.00	45.58
78	NE	ARG	Α	615	29.827	49.226	56.142	1.00	49.04
79	CZ	ARG	Α	615	29.151	48.769	57.151	1.00	51.81
80	NH1	ARG	Α	615	29.164	47.437	57.427	1.00	50.76
81	NH2	ARG	A	615	28.473	49.652	57.883	1.00	51.85
82	С	ARG	Α	615	31.694	51.886	52.150	1.00	45.54
83	0	ARG	Α	615	30.737	52.603	52.357	1.00	47.25
84	N	GLN	Α	616	32.035	51.399	50.944	1.00	45.88
85	CA	GLN	Α	616	31.366	51.824	49.681	1.00	46.97
86	CB	GLN	Α	616	32.323	52.657	48.734	1.00	47.24
87	CG	GLN	Α	616	33.258	53.608	49.475	1.00	49.82
88	CD	GLN			34.200	54.437	48.588	1.00	55.54
89	OE1	GLN			35.203	53.909	48.073		56.72
90	NE2	GLN	Α	616	33.889	55.770	48.428	1.00	56.51
91	C	GLN			30.597	50.752	48.848		46.63
92	0	GLN			29.448	50.970	48.361		48.68
93	N	LYS			31.167	49.598	48.678	1.00	
94	CA	LYS			30.497	48.628	47.857	1.00	
95	CB	LYS	A	617	30.835	48.787	46.331	1.00	44.70

FIGURE 3BA (Cont.)

Α	В	С	D	E	F	G	Н	I	J
96	CG	LYS	7	617	32.399	48.959	45.944	1 00	48.09
97	CD	LYS			32.768	48.759	44.391		58.41
98	CE	LYS			34.285	49.300	44.085		60.72
99	NZ	LYS			35.073	48.944	42.813		59.09
100	C			617	31.019	47.331	48.370		43.38
101	0			617	32.139	47.331	48.834		42.92
101	N			618	30.126	46.333	48.379		42.86
102	CA			618	30.376	44.945	48.657		41.23
103	CB			618	29.070	44.146	48.522		39.95
105					29.426	42.622	48.582		40.13
105		VAL			28.147	44.503	49.610		42.60
107	C			618	31.203	44.381	47.543		40.46
108	0			618	30.854	44.667	46.392		42.70
109	N			619	32.237	43.567	47.809		37.69
	CA			619	33.059	43.022	46.731		33.98
110	CB			619	34.521	43.786	46.731		36.65
111	CG1			619	35.584	43.780	47.540		31.94
112	CD1			619	36.383	44.380	48.493		29.73
113	CG2			619	34.380	45.336	46.302		31.41
114	CG2			619	33.357	41.588	46.302		33.91
115					34.185	41.024	46.280		35.83
116	O N			619		40.970	47.989		32.82
117	N Ca			620	32.752	39.577	48.271		32.89
118	CA C			620 620	33.039	39.194	49.553		32.89
119				620	31.714	39.194	50.177		30.70
120	O N			621	32.511	37.954	49.897		34.15
121	N				31.818	37.384	51.019		35.78
122 123	CA CB			621 621	30.777	36.453	50.533		35.78
	C			621	32.833	36.551	51.687		37.56
124 125	0			621	33.491	35.782	51.007		39.38
126	N			622	33.026	36.691	52.986		38.91
127	CA			622	34.006	35.848	53.611		38.65
128	C			622	33.398	34.928	54.575		39.55
129	0			622	32.173	34.902	54.796		36.11
130	N	GLU			34.293	34.225	55.272		41.01
131	CA	GLU			33.843	33.363	56.342		41.61
132	CB	GLU			35.046	32.793	57.068		43.27
133		GLU			34.682				50.78
134	CD			623		31.063	58.780		65.56
135		GLU			36.962				64.79
136	OE2			623	35.592				72.34
137	C			623	32.965		57.417		40.39
138	0			623		33.457	57.987		38.12
139	N			624	33.265	35.347	57.758		37.75
140	CA			624	32.522	35.965	58.889		36.41
141	CB			624	33.506	36.538	59.933		37.60
142	CG			624	34.593	35.546	60.354		34.22
143		PHE			34.285	34.584	61.169		32.75
144		PHE				33.643			42.16
145	CZ			624		33.666			37.78
146		PHE				34.594			37.66
147		PHE				35.571			37.30
					-	· - · -			

FIGURE 3AP LECEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

į	A	В	С	D	E	F	G	Н	I	J
	2057	N	ALA	R	602	61.588	-1.705	97.096	1.00	75.62
	2058	CA	ALA			61.031	-2.970	96.546	1.00	76.68
	2059	CB	ALA			61.665	-3.292	95.199		76.47
	2060	C	ALA			61.337	-4.080	97.519		77.44
	2061	o	ALA			61.332	-5.311	97.156	1.00	75.75
	2062	N	LYS			61.635	-3.605	98.744	1.00	77.75
	2063	CA	LYS			62.173	-4.417	99.861	1.00	77.56
	2064	CB	LYS			63.425	-3.748	100.411	1.00	78.96
	2065	CG	LYS			63.212	-2.282	100.938	1.00	78.12
	2066	CD	LYS			62.779		102.422	1.00	78.99
	2067	CE	LYS			63.952		103.426	1.00	79.93
	2068	NZ	LYS		603	64.536		103.573	1.00	79.82
	2069	C	LYS			61.103		100.921	1.00	76.81
	2070	0	LYS			61.315		102.072	1.00	75.16
	2071	N	PHE			59.938		100.457	1.00	76.03
	2072	CA	PHE			58.711		101.207	1.00	74.92
	2073	CB	PHE			58.102		100.991	1.00	76.05
	2074	CG	PHE		604	58.700		101.857	1.00	78.39
	2075	CD1	PHE		604	58.564		103.231	1.00	
	2076	CE1	PHE		604	59.115		104.059		84.10
	2077	CZ	PHE		604	59.854		103.511		81.74
	2078	CE2	PHE		604	60.017		102.144		82.47
	2079	CD2	PHE		604	59.448	-0.503	101.312		81.05
	2080	C	PHE		604	57.783		100.707	1.00	73.54
	2081	0		В	604	56.553	-4.941	100.826	1.00	73.46
	2082	N	THR		605	58.368	-6.069	100.190	1.00	
	2083	CA	THR			57.496	-7.068	99.640		68.96
	2084	СВ	THR			57.540	-6.922	98.163		68.75
	2085	OG1	THR			57.203	-8.191	97.632	1.00	
	2086	CG2	THR			58.991	-6.774	97.722		71.15
	2087	C	THR			57.874	-8.494	99.969		65.74
	2088	ō	THR			59.000	-8.868	99.864		66.65
	2089	N	THR			56.897		100.339		61.47
	2090	CA	THR			57.083	-10.702			56.89
	2091	СВ	THR			55.818	-11.150	101.234		58.04
	2092	OG1	THR			55.636	-10.407			53.91
	2093	CG2	THR			55.854	-12.662	101.579		56.07
	2094	C	THR	_			-11.402	99.182		55.32
	2095	ō	THR				-11.139	98.285		55.18
	2096	N	GLU				-12.330	99.008		52.87
	2097	CA	GLU				-13.077	97.771		48.83
	2098	CB	GLU				-13.585	97.546		50.19
	2099	CG	GLU			59.720		96.488		49.52
:	2100	CD	GLU				-14.069	95.132		53.13

FIGURE 1

Amino acid sequence for full length human wild type EPHA2 [SEQ ID NO: 1] (Residues 596-900 are underlined)

MELQAARACFALLWGCALAAAAAAQGKEVVLLDFAAAGGELGWLTHPYGK	50
GWDLMQNIMNDMPIYMYSVCNVMSGDQDNWLRTNWVYRGEAERNNFELNF	100
TVRDCNSFPGGASSCKETFNLYYAESDLDYGTNFQKRLFTKIDTIAPDEI	150
TVSSDFEARHVKLNVEERSVGPLTRKGFYLAFQDIGACVALLSVRVYYKK	200
CPELLQGLAHFPETIAGSDAPSLATVAGTCVDHAVVPPGGEEPRMHCAVD	250
GEWLVPIGQCLCQAGYEKVEDACQACSPGFFKFEASESPCLECPEHTLPS	300
PEGATSCECEEGFFRAPQDPASMPCTRPPSAPHYLTAVGMGAKVELRWTP	350
PQDSGGREDIVYSVTCEQCWPESGECGPCEASVRYSEPPHGLTRTSVTVS	400
DLEPHMNYTFTVEARNGVSGLVTSRSFRTASVSINQTEPPKVRLEGRSTT	450
SLSVSWSIPPPQQSRVWKYEVTYRKKGDSNSYNVRRTEGFSVTLDDLAPD	500
TTYLVQVQALTQEGQGAGSKVHEFQTLSPEGSGNLAVIGGVAVGVVLLLV	550
LAGVGFFIHRRRKNQRARQSPEDVYFSKSEQLKPLKTYVDPHTYE <u>DPNQA</u>	600
VLKFTTEIHPSCVTRQKVIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKA	650
GYTEKQRVDFLGEAGIMGQFSHHNIIRLEGVISKYKPMMIITEYMENGAL	700
DKFLREKDGEFSVLQLVGMLRGIAAGMKYLANMNYVHRDLAARNILVNSN	750
LVCKVSDFGLSRVLEDDPEATYTTSGGKIPIRWTAPEAISYRKFTSASDV	800
WSFGIVMWEVMTYGERPYWELSNHEVMKAINDGFRLPTPMDCPSAIYQLM	850
MQCWQQERARRPKFADIVSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	900
SEGVPFRTVSEWLESIKMQQYTEHFMAAGYTAIEKVVQMTNDDIKRIGVR	950
LPGHOKRIAYSLLGLKDQVNTVGIPI	976

FIGURE 1A

Human cDNA sequence encoding residues 596-900 of EPHA2 [SEQ ID NO: 2]

GACCCCAACCAGGCTGTGTTGAAGTTCACTACCGAGATCCATCC	50
TGTCACTCGGCAGAAGGTGATCGGAGCAGGAGAGTTTGGGGAGGTGTACA	100
AGGGCATGCTGAAGACATCCTCGGGGAAGAAGGAGGTGCCGGTGGCCATC	150
AAGACGCTGAAAGCCGGCTACACAGAGAAGCAGCGAGTGGACTTCCTCGG	200
CGAGGCCGGCATCATGGGCCAGTTCAGCCACCACAACATCATCCGCCTAG	250
AGGGCGTCATCTCCAAATACAAGCCCATGATGATCATCACTGAGTACATG	300
GAGAATGGGGCCCTGGACAAGTTCCTTCGGGAGAAGGATGGCGAGTTCAG	350
CGTGCTGCAGCTGGTGGGCATGCTGCGGGGCATCGCAGCTGGCATGAAGT	400
ACCTGGCCAACATGAACTATGTGCACCGTGACCTGGCTGCCCGCAACATC	450
CTCGTCAACAGCAACCTGGTCTGCAAGGTGTCTGACTTTGGCCTGTCCCG	500
CGTGCTGGAGGACCCCGAGGCCACCTACACCACCAGTGGCGGCAAGA	550
TCCCCATCCGCTGGACCGCCCCGGAGGCCATTTCCTACCGGAAGTTCACC	600
TCTGCCAGCGACGTGTGGAGCTTTGGCATTGTCATGTGGGAGGTGATGAC	650
CTATGGCGAGCGGCCCTACTGGGAGTTGTCCAACCACGAGGTGATGAAAG	700
CCATCAATGATGGCTTCCGGCTCCCCACACCCATGGACTGCCCCTCCGCC	750
ATCTACCAGCTCATGATGCAGTGCTGGCAGCAGGAGCGTGCCCGCCC	800
CAAGTTCGCTGACATCGTCAGCATCCTGGACAAGCTCATTCGTGCCCCTG	850
ACTCCCTCAAGACCCTGGCTGACTTTGACCCCCGCGTGTCTATCCGGCTC	900
CCCAGCACGAGCGGC	915

Amino acid sequence for residues 596-900 of EPHA2 with a cleavable (rTev) N-terminal 6x-histidine tag [SEQ ID NO: 3] (6x-histidine tag and cleavage site are underlined)

MSYYHHHHHHDYDIPTTENLYFQGAMGSDPNQAVLKFTTEIHPSCVTRQK	50
VIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKAGYTEKQRVDFLGEAGIM	100
GQFSHHNIIRLEGVISKYKPMMIITEYMENGALDKFLREKDGEFSVLQLV	150
GMLRGIAAGMKYLANMNYVHRDLAARNILVNSNLVCKVSDFGLSRVLEDD	200
PEATYTTSGGKIPIRWTAPEAISYRKFTSASDVWSFGIVMWEVMTYGERP	250
YWELSNHEVMKAINDGFRLPTPMDCPSAIYQLMMQCWQQERARRPKFADI	300
VSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	333

FIGURE 3

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number' (SEQ ID NO: 1), (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	В	С	D	E	F	G	Н	I	J
1	N	ALA	Α	605	47.239	45.529	67.448	1.00	51.83
2	CA	ALA	Α	605	46.929	45.860	66.049	1.00	52.40
3	CB	ALA	Α	605	45.751	44.876	65.490		51.40
4	С	ALA	Α	605	46.433	47.259	66.307	1.00	51.78
5	0	ALA	A	605	46.252	47.630	67.422	1.00	52.61
6	N	THR	Α	606	46.218	48.048	65.302	1.00	51.19
7	CA	THR	Α	606	45.719	49.337	65.564	1.00	49.98
8	CB	THR	Α	606	46.128	50.120	64.454	1.00	48.98
9	OG1	THR	Α	606	47.553	50.041	64.401	1.00	50.88
10	CG2	THR	Α	606	45.766	51.541	64.651	1.00	48.25
11	С	THR	Α	606	44.201	49.397	65.650	1.00	50.57
12	0	THR	Α	606	43.487	48.868	64.787	1.00	51.60
13	N	GLU	Α	607	43.680	50.086	66.646	1.00	49.68
14	CA	GLU	Α	607	42.264	50.182	66.717	1.00	47.97
15	CB	GLU	Α	607	41.796	50.123	68.130	1.00	47.41
16	CG	GLU	Α	607	40.323	50.414	68.279	1.00	50.07
17	CD	GLU	Α	607	39.394	49.230	68.074	1.00	39.82
18	OE1	GLU	А	607	39.796	48.072	68.195	1.00	38.52
19	OE2	GLU	Α	607	38.260	49.515	67.856	1.00	41.61
20	C	GLU	А	607	41.841	51.347	65.971	1.00	48.16
21	0			607	42.392	52.398	66.162		48.74
22	N	ILE	Α	608	40.955	51.146	64.963		50.14
23	CA			608	40.531	52.309	64.228		49.42
24	CB	ILE	Α	608	41.128	52.517	62.742		51.19
25	CG1			608	40.066	52.886	61.752		49.45
26	CD1			608	39.259		61.615		60.72
27	CG2			608	42.168	51.494	62.300		47.67
28	С			608	39.135	52.787	64.481		51.43
29	0			608	38.254	52.049	64.879		51.22
30	N			609	38.983	54.090	64.361		53.40
31	CA			609	37.727	54.745	64.674		55.30
32	CB			609	37.938	56.203	65.196	1.00	
33	CG			609	36.715	56.776	65.835		60.02
34	ND1	HIS			36.486	56.686	67.186		62.57
35	CE1	HIS			35.313	57.221	67.471		62.48
36	NE2	HIS			34.764	57.635	66.348		63.53
37	CD2	HIS			35.606	57.345	65.301		62.09
38	C	HIS			36.701	54.718	63.557		53.34
39	0	HIS			36.943	55.109	62.474		55.03
40	N			610	35.517	54.263	63.854		52.90
41	CA			610	34.533	54.113	62.805		53.20
42	CB			610	33.246	53.864	63.591		52.67
43	CG	PRO	Α	610	33.753	53.087	64.713	1.00	50.94

FIGURE 3A

A	В	С	D	E	F	G	Н	I	J
44	CD	PRO	Α	610	35.069	53.682	65.133	1.00	52.08
45	С	PRO	A	610	34.421	55.273	61.903	1.00	52.69
46	0	PRO	А	610	33.935	55.146	60.793	1.00	55.21
47	N	SER			34.789	56.418	62.391	1.00	52.17
48	CA	SER	Α	611	34.546	57.584	61.639	1.00	52.33
49	CB	SER	Α	611	34.694	58.833	62.562	1.00	54.93
50	OG	SER	А	611	35.822	58.723	63.443	1.00	49.81
51	Ċ	SER	Α	611	35.579	57.611	60.552	1.00	52.77
52	0	SER	Α	611	35.394	58.256	59.545	1.00	54.01
53	N	CYS	Α	612	36.679	56.915	60.701	1.00	49.87
54	CA	CYS	Α	612	37.633	57.083	59.642	1.00	51.06
55	CB	CYS	Α	612	39.044	56.889	60.169	1.00	50.65
56	SG	CYS	А	612	39.193	57.805	61.702	1.00	55.75
57	C	CYS	Α	612	37.445	56.214	58.426	1.00	49.07
58	0	CYS	Α	612	38.215	56.286	57.479	1.00	48.12
59	N	VAL	Α	613	36.470	55.349	58.497	1.00	49.20
60	CA	VAL	Α	613	36.329	54.361	57.471		48.42
61	CB	VAL	А	613	36.130	52.976	58.087		49.58
62	CG1	VAL	Α	613	35.493	52.026	57.030		46.32
63	CG2	VAL	Α	613	37.477	52.423	58.651		46.61
64	С	VAL	A	613	35.039	54.652	56.779		47.49
65	0	VAL			34.080	55.078	57.401		46.54
66	N	THR			34.976	54.426	55.496		46.87
67	CA	THR	Α	614	33.674	54.449	54.961		47.76
68	CB	THR			33.230	55.839	54.547		48.10
69	OG1	THR	A	614	32.501	55.759	53.312		53.74
70	CG2	THR			34.430	56.804	54.383		48.56
71	C	THR			33.479	53.362	53.956		47.36
72	0	THR			34.145	53.317	52.971		49.44
73	N	ARG			32.519	52.496	54.192		46.37
74	CA	ARG			32.356	51.360	53.352		44.80
75	CB	ARG			31.323	50.464	53.993		43.89
76	CG	ARG			31.817	49.366	54.921		44.82
77	CD	ARG			30.699	48.434	55.297		45.58
78	NE	ARG			29.827	49.226	56.142		49.04
79	CZ	ARG			29.151	48.769	57.151		51.81
80		ARG			29.164	47.437	57.427		50.76 51.85
81		ARG			28.473	49.652	57.883		45.54
82	C	ARG			31.694	51.886	52.150		47.25
83	0	ARG			30.737	52.603	52.357		
84	N	GLN			32.035	51.399	50.944		45.88 46.97
85	CA	GLN			31.366	51.824 52.657	49.681 48.734		47.24
86	CB	GLN			32.323				49.82
87	CG	GLN			33.258	53.608	49.475 48.588		55.54
88	CD OF1	GLN GLN			34.200 35.203	54.437 53.909	48.073		56.72
89 90	NE2	GLN			33.889	55.770	48.428		56.51
	NE2 C	GLN			30.597	50.752	48.848		46.63
91 92	0 .	GLN			29.448	50.752	48.361		48.68
	N O	LYS			31.167		48.678		44.77
93 94	CA	LYS					47.857		44.21
95	CB	LYS			30.437		46.331		44.70
23	CD	פזת	А	017	50.055	40.707	20.001	1.00	

FIGURE 3B

A	В	C	D	E		F	G	H	I	J
96	CG	T.VC	7	617		32.399	48.959	45.944	1 00	48.09
97	CD			617		32.768	48.759	44.391		58.41
98	CE			617		34.285	49.300	44.085		60.72
99	NZ			617		35.073	48.944	42.813		59.09
100	C			617		31.019	47.331	48.370		43.38
101	0			617		32.139	47.297	48.834		42.92
101	N			618		30.126	46.333	48.379		42.86
	CA			618		30.126	44.945	48.657		41.23
103	CB			618		29.070	44.146	48.522		39.95
104	CG1	VAL				29.426	42.622	48.582		40.13
105	CG1	VAL				28.147	44.503	49.610		42.60
106							44.303	47.543		40.46
107	C			618		31.203	44.561	46.392		42.70
108	0			618		30.854	43.567	47.809		37.69
109	N			619		32.237				
110	CA			619		33.059	43.022	46.731		33.98
111	CB			619		34.521	43.786	46.495		36.65
112	CG1			619		35.584	43.320	47.540		31.94
113	CD1			619		36.383	44.380	48.493		29.73
114	CG2			619		34.380	45.336	46.302		31.41
115	C			619		33.357	41.588	46.995		33.91
116	0			619		34.185	41.024	46.280		35.83
117	N			620		32.752	40.970	47.989		32.82
118	CA			620		33.039	39.577	48.271		32.89
119	C			620		32.373	39.194	49.553		32.89
120	0			620		31.714	39.949	50.177		30.70
121	N			621		32.511	37.954	49.897		34.15
122	CA			621		31.818	37.384	51.019		35.78
123	CB	ALA				30.777	36.453	50.533		35.84
124	C			621		32.833	36.551	51.687		37.56
125	0			621		33.491	35.782	51.007		39.38
126	N			622		33.026	36.691	52.986		38.91
127	CA			622		34.006	35.848	53.611		38.65
128	C	GLY				33.398	34.928	54.575		39.55
129	0	GLY				32.173	34.902	54.796		36.11
130	N	GLU				34.293	34.225	55.272		41.01
131	CA	GLU				33.843	33.363	56.342		41.61
132	CB	GLU				35.046	32.793	57.068		43.27
133	CG	GLU				34.682				50.78
134	CD	GLU				35.838		58.780		65.56
135		GLU				36.962	31.030	58.200		64.79
136	OE2	GLU				35.592	30.422	59.836		72.34
137	C	GLU				32.965	34.088	57.417		40.39
138	0			623	•	32.055	33.457	57.987		38.12
139	N			624		33.265	35.347	57.758		37.75
140	CA			624		32.522	35.965	58.889		36.41
141	CB			624		33.506	36.538	59.933		37.60
142	CG			624		34.593	35.546	60.354		34.22
143		PHE				34.285	34.584	61.169		32.75
144		PHE				35.256	33.643	61.527		42.16
145	CZ			624		36.568	33.666	61.022		37.78
146				624			34.594			37.66
147	CD2	PHE	A	624		35.861	35.571	59.805	1.00	37.30

FIGURE 3C

A	В	С	D	E	F		G	Н	I	J
148	C	PHE	Α	624	31.5	69 37.	.066	58.437	1.00	35.68
149	0	PHE	Α	624	30.8		.739	59.261	1.00	36.44
150	N	GLY	Α	625	31.5	57, 37	.336	57.140	1.00	35.15
151	CA	GLY	Α	625	30.7	31 38.	.445	56.714	1.00	32.08
152	C	GLY	Α	625	31.1	64 39	.011	55.423	1.00	32.29
153	0	GLY	A	625	32.1	77 38	.633	54.858	1.00	32.00
154	N	GLU	Α	626	30.4	22 39	.990	54.988	1.00	33.82
155	CA	GLU	A	626	30.7	10 40	.519	53.695	1.00	37.80
156	CB	GLU	Α	626	29.5	34 41	.289	53.103		36.83
157	CG			626	28.3		.298	52.839		42.38
158	CD			626	27.3		.941	51.992		45.04
159	OE1	GLU			27.2		.680	50.777		47.93
160	OE2	GLU			26.6		.773	52.553		43.41
161	C			626	31.8		.377	53.719		37.16
162	0			626	32.2		.878	54.803		35.84
163	N			627	32.4		.552	52.508		35.91
164	CA			627	33.7		.268	52.392		34.05
165	CB			627	34.8		.340	51.861		36.58
166	CG1	VAL			36.2		.135	51.691		30.17
167	CG2	VAL			34.9		.244	52.740		33.27
168	C			627	33.3		.380 .157	51.461 50.568		34.18 31.95
169 170	O N			627 628	32.6 33.9		. 575	51.680		33.62
171	CA			628	33.6		.746	50.948		33.35
172	CB			628	32.8		.766	51.894		35.70
173	CG			628	31.5		.398	52.411		35.23
174	CD1			628	31.3		.529	53.497		34.62
175	CE1			628	30.0		.215	53.976		36.28
176	CZ			628	28.9		.759	53.348		39.83
177	OH			628	27.6		.479	53.748		41.33
178	CE2			628	29.0		.582	52.266		43.12
179	CD2			628	30.3	97 46	.941	51.826	1.00	40.98
180	C	TYR	Α	628	34.8	90 46	.407	50.597	1.00	33.72
181	0	TYR	Α	628	35.9	38 46	.184	51.223	1.00	35.69
182	N	LYS	Α	629	34.7	49 47	.365	49.743	1.00	33.77
183	CA	LYS	Α	629	35.7	92 48	.236	49.369	1.00	36.45
184	CB			629	35.6	13 48	.688	47.939		36.34
185	CG	LYS	Α	629	36.6	92 49	.598	47.624		41.68
186	CD			629	36.2		.858	47.072		45.46
187	CE	LYS	Α	629	37.4		.809	46.890		51.36
188	NZ			629	36.9		.283	46.736		49.95
189	С			629	35.4		.455	50.046		37.55
190	0			629	34.2		.740	50.227		37.87
191	N			630	36.4		.286	50.355		41.21
192	CA			630	36.0		.559	50.912		42.33
193	C			630	37.2		.450	51.067		44.89
194	0			630	38.2		.287	50.392		45.71
195	N			631	37.0		.363	52.008		46.92
196	CA	MET			38.0		.443	52.136		48.84 49.65
197	CB			631	37.3		.734	51.608		51.92
198	CG			631	37.1		.731	50.070		57.95
199	SD	MET	A	631	38.7	4/ 55	.249	49.171	1.00	31.33

FIGURE 3D

A	В	C	D	E		F	. (G		H	I	J
			_									
200	CE	MET				9.478	56.			727		56.76
201	C	MET				3.379	54.			587		49.23
202	0	MET				7.493	54.			462		47.16
203	Ŋ	LEU				9.696	54.			828		47.01
204	CA			632		0.144	54.			148		48.50
205	CB	LEU				1.204	53.			531		46.95
206	CG	LEU				1.924	54.			805		47.11
207	CD1	LEU				0.936	53.			902		45.89
208	CD2	LEU				3.172	53.				1.00	
209	C	LEU				0.680	56.			221		50.08
210	0	LEU				1.388	56.			323		47.85
211	N	ALA				0.279	57.			256		52.44
212	CA	ALA				0.873	58.			388		56.35
213	CB	ALA				9.848	59.			836		55.50
214	C	ALA				1.842	58.			445		56.34
215	0	ALA				1.406	57.			493		58.62
216	N	ALA				3.136	58.			224		57.84
217	CA	ALA				3.920	57.			415		61.35
218	CB	ALA				5.364	57.			115		62.22
219	C	ALA				3.771	59.			222	1.00	
220	0			634		4.422	60.	208		850		64.38
221	N			638		3.383	64.			993		78.26
222	CA	ALA				1.752	64.			359		79.12
223	CB	ALA				5.788	63.			237		78.95
224	C	ALA				1.822	63.			872		79.32
225	0	ALA				5.141	64.			006		
226	N	ALA	Α	639	4	4.531	62.			589	1.00	78.59
227	CA	ALA				1.620	61.		53.	238	1.00	77.38
228	CB	ALA				5.119	61.		52.	875	1.00	78.65
229	C			639		3.843	60.			247	1.00	75.52
230	0	ALA	Α	639	4	1.050	59.			155		75.87
231	N			640		2.935	60.			273	1.00	71.51
232	CA	GLU				1.968	59.			171		66.84
233	CB	GLU				0.701	59.			433		66.51
234	CG	GLU				9.483	58.			713		68.84
235	CD	GLU				3.106	59.			585	1.00	
236	OE1	GLU				7.834	60.			511	1.00	
237	OE2	GLU				7.274				561		70.47
238	C	GLU				2.571	58.			379		63.66
239	0			640		3.179				363		64.69
240	N	VAL				2.394	56.			807		60.16
241	CA	VAL				3.028	55.			100		55.19
242	CB	VAL				1.352	55.			777		54.62
243	CG1	VAL				1.223	54.			749		50.91
244	CG2	VAL				5.363	55.			767		56.67
245	C	VAL				2.102	54.			931		52.53
246	0			641		1.378				812		55.11
247	N			642		2.105				767		51.34
248	CA	PRO				1.271	52.			477		47.14
249	CB	PRO				1.664				064		47.64
250	CG	PRO				2.633				544		50.33
251	CD	PRO	A	642	42	2.943	54.	475	48.	637	1.00	50.56

FIGURE 3E

A	В	С	D	E	F	G	Н	I	J
252	С	PRO	Δ	642	41.625	51.589	50.367	1.00	45.19
253	0			642	42.816	51.373	50.765		44.61
254	N			643	40.636	50.779	50.710		40.92
255	CA			643	40.925	49.716	51.646	1.00	
256	CB			643	40.652	50.209	53.117		37.96
257	CG1			643	41.889	50.869	53.733		39.75
258	CG2	VAL			39.377	51.186	53.225	1.00	
259	C			643	39.921	48.664	51.373		36.92
260	0			643	38.827	48.941	50.848		38.74
261	N			644	40.226	47.464	51.769		34.90
262	CA			644	39.217	46.411	51.722		34.08
263	CB			644	39.858	45.092	51.412		31.97
264	C			644	38.726	46.373	53.179		35.58
265	0			644	39.526	46.373	54.096		30.86
							53.393		36.25
266	N			645 645	37.443	45.968			34.97
267	CA				36.922	45.950	54.744 54.876		35.85
268	CB			645	35.932	47.080			
269	CG1			645	36.577	48.336	54.488		37.94
270	CD1			645	35.489	49.480	54.224		39.26
271	CG2			645	35.314	47.127	56.304		32.71
272	C			645	36.201	44.682	55.066		33.98
273	0			645	35.113	44.491	54.584	1.00	
274	N			646	36.714	43.846	55.922		34.87
275	CA			646	36.008	42.632	56.289		38.18
276	CB			646	37.040	41.499	56.633		39.75
277	CG			646	37.905	41.096	55.427		44.65
278	CD	LYS			38.718	39.873	55.721		47.74
279	CE	LYS			38.775	38.957	54.557		56.44
280	ΝZ	LYS			40.016	39.325	53.698		67.82
281	C	LYS			35.078	42.871	57.482	1.00	
282	0			646	35.524	43.217	58.526		39.11
283	N			647	33.779	42.703	57.344		38.53
284	CA			647	32.898	42.869	58.518		35.17
285	CB			647	31.620	43.563	58.086		35.95
286	OG1	THR			30.886	42.779	57.136		31.75
287	CG2	THR			31.977	44.751	57.224		26.19
288	C			647	32.581	41.580	59.205		35.41
289	0	THR			32.741	40.482	58.693		36.20
290	N	LEU			32.208	41.704	60.429		35.38
291	CA			648	31.915	40.572	61.187		37.01
292	CB			648	32.612	40.708	62.523		36.29
293	CG	LEU			32.176	39.634	63.510		34.38
294	CD1	LEU			32.349	38.265	63.066		33.21
295	CD2	LEU			32.938	39.707	64.670		38.96
296	С	LEU			30.383	40.645	61.334		39.65
297	0	LEU			29.873	41.630	61.869		41.32
298	N	LYS			29.631	39.670	60.813		39.93
299	CA	LYS			28.175	39.764	60.832		38.04
300	CB	LYS			27.610	38.564	60.128		38.58
301	CG	LYS			27.766	37.309			38.14
302	CD	LYS			27.679		59.889		35.47
303	CE	LYS	Α	649	27.535	34.883	60.524	1.00	35.35

FIGURE 3F

A	В	С	D	E		F		G		Н	I	J
304	NZ	LYS	Α	649	2	7.499	33	.710	59	.600	1.00	36.16
305	С	LYS	Α	649	2	7.630	39	.998	62	.226	1.00	38.13
306	0	LYS	Α	649	2	8.217	39	.517	63	.181	1.00	38.78
307	N	ALA	Α	650	2	6.642	40	.900	62	.370	1.00	38.37
308	CA	ALA	Α	650	2	6.009	41	.267	63	.688	1.00	38.30
309	CB	ALA	Α	650	2.	4.721	41	.954	63	.443	1.00	37.99
310	C	ALA	Α	650	2.	5.680	39	.928	64	.183	1.00	38.32
311	0	ALA	Α	650	2.	5.410	39	.138	63	.320	1.00	40.75
312	N	GLY	Α	651	2.	5.632	39	.493	65	.416	1.00	35.55
313	CA	GLY	Α	651	2	5.195	3.8	.071	65	.179	1.00	36.67
314	C	GLY	Α	651	2	6.171	36	.916	65	.234	1.00	33.22
315	0	GLY	Α	651	2	5.899	35	.767	65	.646	1.00	30.70
316	N	TYR	Α	652	2	7.390	37	.294	65	.039	1.00	34.28
317	CA	TYR	Α	652	2	8.455	36	.416	65	.446	1.00	36.25
318	CB	TYR	Α	652	2	9.684	37	.205	65	.494	1.00	38.05
319	CG	TYR	Α	652	2	9.668	38	.292	66	.484	1.00	38.76
320	CD1	TYR	Α	652	3	0.221	38	.086	67	.745	1.00	36.74
321	CE1	TYR	Α	652	3	0.242	39	.091		.684		34.51
322	CZ	TYR			2	9.778	40	.325		.329		40.27
323	OH	TYR	А	652	2	9.893	41	.245		.291		42.40
324	CE2	TYR	Α	652	2	9.178		.584		.038		34.15
325	CD2	TYR	Α	652		9.169		.556		.141		38.47
326	C	TYR	Α	652	2	8.386		.850		.803		35.31
327	0	TYR	А	652	2	7.919		.531		.696		34.45
328	N	THR	Α	653	2	8.961		.652		.947		35.94
329	CA	THR	Α	653		9.209		.999		.234		36.94
330	CB			653		9.248		.522		.183		37.69
331	OG1			653		0.427		.201		.433		40.83
332	CG2			653		8.007		.792		.363		32.24
333	C			653		0.595		.418		.718		37.14
334	0			653		1.347		.985		.015		37.03
335	N			654		0.831		.210		.998		37.12
336	CA			654		2.094		.484		.674		37.20
337	CB			654		2.074		.802		.025		34.84
338	CG			654		3.380		.188		.705		44.32
339	CD			654		3.571		.731		.609		48.08
340		GLU				2.591		.470		.366		54.40
341		GLU				4.675		.206		2.771		46.32
342	C			654		3.316		.880		.890		35.96
343	0			654		4.306		.579		.620		33.58
344	N			655		3.161		.605		577		35.57
345	CA			655		4.030		.857		3.747		39.28
346	CB			655		3.532		.394		.482		39.74
347	CG			655		4.682		.481		0.003		46.57
348	CD			655		4.375		.446		.854		53.64
349	CE			655		5.674		.584		3.374		58.92
350	NZ			655		7.147		.174		3.350	1.00	
351	C			655		4.326		.574		.379		38.72
352	0			655		5.481		.624		.012		41.81
353	N			656		3.329		.111		.678		35.08
354	CA			656		3.583		.809		5.411		36.08
355	CB	GLN	Α	656	3	2.355	34	.070	64	.590	1.00	32.82

FIGURE 3G

A	В	.C	D	E	F	G	Н	I	J
356	CG	GLN	А	656	31.709	32.793	64.216	1.00	35.27
357	CD			656.	30.255	32.982	63.707		37.96
358	OE1	GLN	A	656	29.471	33.846	64.157	1.00	30.18
359	NE2	GLN	Α	656	29.948	32.217	62.693	1.00	42.57
360	C	GLN	Α	656	34.305	35.111	65.659	1.00	35.54
361	0	GLN	Α	656	35.196	35.485	64.899	1.00	35.47
362	N	ARG	Α	657	33.951	35.722	66.760	1.00	35.39
363	CA	ARG	Α	657	34.557	36.985	67.147	1.00	39.00
364	CB	ARG	Α	657	33.923	37.539	68.413	1.00	37.06
365	CG	ARG	Α	657	34.401	38.841	68.811	1.00	40.49
366	CD	ARG	Α	657	34.033	39.137	70.269		41.44
367	NE	ARG	Α	657	34.843	40.262	70.614		54.97
368	CZ	ARG	Α	657	35.982	40.205	71.383	1.00	
369	NH1	ARG			36.451	39.051	71.945		43.49
370	NH2	ARG			36.616	41.349	71.556	1.00	
371	C			657	36.017	36.717	67.311	1.00	
372	0			657	36.826	37.240	66.592		37.52
373	N			658	36.331	35.771	68.150		42.72
374	CA			658	37.722	35.481	68.321		45.25
3,75	CB	VAL			37.957	34.577	69.517		47.74
376	CG1	VAL			39.291	33.787	69.368		48.43
377	CG2	VAL			37.935	35.483	70.791		49.98
378	C	VAL			38.449	35.036	67.044	1.00	
379	0	VAL			39.466	35.669	66.720		44.99
380	N			659	37.913	34.045	66.299		42.92
381	CA	ASP			38.561	33.655	65.043		41.99
382	CB	ASP			37.891	32.498	64.307		41.26 45.94
383	CG	ASP			37.826 37.109	31.278	65.177 64.847		46.31
384 385	OD1	ASP ASP			38.451	30.301 31.252	66.249		43.77
386	C	ASP			38.683	34.857	64.176	1.00	
387	0	ASP			39.687	35.012	63.586		36.58
388	N			660	37.703	35.756	64.220		38.73
389	CA			660	37.765	36.881	63.312		39.49
390	CB			660	36.385	37.556	63.203	1.00	37.46
391	CG			660	36.343	38.830	62.388	1.00	33.56
392		PHE			36.342	40.047	62.976		32.33
393		PHE				41.209	62.257		28.65
394	CZ			660	36.136	41.248	60.858		24.95
395	CE2	PHE	A	660	36.059	40.060	60.259	1.00	28.98
396	CD2			660	36.099	38.814	61.088	1.00	32.15
397	С			660	38.897	37.885	63.675		39.32
398	0			660	39.584	38.276	62.825	1.00	38.41
399	N	LEU	Α	661	39.061	38.276	64.928	1.00	40.15
400	CA	LEU	Α	661	40.011	39.306	65.232	1.00	42.07
401	CB	LEU			39.711	39.915	66.582	1.00	43.38
402	CG			661	38.437	40.774	66.709	1.00	43.55
403	CD1	LEU	А	661	38.306	41.372	68.133	1.00	39.97
404	CD2	LEU	Α	661 .	38.580	41.902	65.756	1.00	37.68
405	C	LEU	А	661	41.347	38.552	65.294		41.94
406	0	LEU	A	661	42.340	39.129			41.62
407	N	GLY	A	662	41.349	37.252	65.485	1.00	39.75

FIGURE 3H

A	В	С	D	E	F	G	Н	I	J
408	CA	GLY	Α	662	42.603	36.635	65.570	1.00	40.93
409	C			662	43.418	36.757	64.273	1.00	43.18
410	0	GLY	Α	662	44.590	37.160	64.286	1.00	42.86
411	N	GLU	Α	663	42.779	36.439	63.154	1.00	42.57
412	CA	GLU	Α	663	43.393	36.553	61.894	1.00	42.39
413	CB	GLU	Α	663	42.379	36.281	60.792	1.00	44.11
414	CG	GLU	Α	663	42.829	36.991	59.480	1.00	48.03
415	CD	GLU	Α	663	42.396	36.230	58.234	1.00	
416	OE1	GLU	Α	663	41.241	35.605	58.330	1.00	52.44
417	OE2			663	43.208	36.292	57.213	1.00	
418	C			663	43.976	37.968	61.741	1.00	
419	0			663	45.090	38.192	61.213		37.63
420	N			664	43.273	38.944	62.230		38.99
421	CA			664	43.939	40.237	62.062		40.23
422	CB			664	42.965	41.347	62.358		41.34
423	C			664	45.114	40.278	63.055	1.00	
424	0			664	46.136	40.873	62.831		39.10
425	N			665	44.989	39.570	64.138	1.00	
426	CA			665	46.087	39.586	65.064		42.63
427	C			665	47.347	39.076	64.355		44.59
428	0			665	48.410	39.610	64.610		45.78
429	N			666	47.200	38.070	63.464 62.941		44.36
430	CA			666	48.295	37.277 36.023	62.510		42.46 44.08
431 432	CB CG1			666 666	47.627 47.247	35.276	63.731		42.77
433	CD1			666	46.394	34.096	63.731	1.00	
434	CG2			666	48.406	35.006	61.565		42.50
435	C			666	48.846	38.081	61.853		41.32
436	0			666	49.986	38.330	61.798		41.39
437	N			667	47.988	38.726	61.143		41.98
438	CA			667	48.371	39.417	59.971	· ·	41.72
439	CB			667	47.073	39.871	59.303		42.41
440	CG			667	47.154	40.885	58.149	1.00	41.60
441	SD	MET	Α	667	45.384	40.798	57.345	1.00	50.77
442	CE			667	44.917	39.215	57.870	1.00	44.36
443	С	MET	Α	667	49.155	40.575	60.497	1.00	42.65
444	0	MET	Α	667	50.088	41.128	59.816	1.00	38.11
445	N	GLY	Α	668	48.790	40.953	61.734	1,.00	42.74
446	CA	GLY	Α	668	49.348	42.203	62.310	1.00	42.47
447	С			668	50.820	42.083	62.677	1.00	40.74
448	0	GLY	А	668	51.552	43.010	62.772	1.00	39.44
449	N	GLN	Α	669	51.241	40.861	62.790		40.10
450	CA	GLN	Α	669	52.563	40.577	63.149	1.00	
451	CB			669	52:547	39.193	63.729	1.00	
452	CG			669	52.011	39.318	65.065		43.35
453	CD			669	51.833	37.999	65.772		53.41
454	OE1	GLN			50.716	37.616	66.048		59.36
455	NE2	GLN			52.917	37.334	66.121	1.00	57.56
456	C			669	53.472	40.657	61.955	1.00	
457	0			669	54.683	40.622	62.152		41.00
458	N		-	670	52.922	40.908	60.729	1.00	
459	CA	PHE	Α	670	53.738	40.932	59.578	1.00	38.18

FIGURE 3I

Α	В	С	D	E	F	G	Н	I	J
460	СВ	PHE	Α	67.0	53.159	9 40.016	58.570	1.00	40.10
461	CG			670	52.990		59.105	1.00	35.26
462	CD1			670	51.962		58.751	1.00	
463	CE1			670	51.803		59.214	1.00	35.47
464	CZ			670	52.720	36.032	59.976	1.00	
465	CE2	PHE			53.818		60.310		40.51
466	CD2	PHE			53.948		59.833	1.00	
467	C			670	53.941		58.974	1.00	
468	Ō			670	53.038		59.012		37.82
469	N			671	55.170		58.485		37.93
470	CA			671	55.327		57.712	1.00	39.08
471	CB			671	55.937		58.533		40.17
472	OG			671	55.915		57.754		43.39
473	С	SER			56.231	L 43.445	56.466	1.00	41.33
474	0	SER			57.490		56.554	1.00	38.64
475	N	HIS	Α	672	55.586	43.358	55.295	1.00	42.48
476	CA	HIS	Α	672	56.279	42.870	54.089	1.00	42.62
477	CB	HIS	Α	672	56.565	41.391	54.190	1.00	42.23
478	CG	HIS	Α	672	57.524	40.981	53.156	1.00	47.30
479	ND1	HIS	Α	672	57.142	40.782	51.825	1.00	46.67
480	CE1	HIS	Α	672	58.240	40.523	51.126	1.00	45.98
481	NE2	HIS	Α	672	59.289	40.519	51.949	1.00	44.11
482	CD2	HIS	Α	672	58.874	40.826	53.214	1.00	45.01
483	C	HIS	Α	672	55.513	3 43.134	52.819	1.00	42.33
484	0	HIS	Α	672	54.388	3 42.761	52.732	1.00	41.57
485	N	HIS	Α	673	56.192	43.697	51.819	1.00	42.80
486	CA	HIS	Α	673	55.610	44.132	50.553	1.00	42.36
487	CB	HIS	Α	673	56.722	44.316	49.548	1.00	38.97
488	CG	HIS	A	673	56.262	2 44.939	48.249	1.00	46.80
489	ND1	HIS	Α	673	55.503	3 46.087	48.211		49.74
490		HIS			55.348		46.956		43.86
491		HIS			55.959		46.172		43.54
492	CD2	HIS			56.496		46.944		42.26
493	C	HIS			54.523		49.883		40.55
494	0	HIS			53.543		49.310		42.61
495	N	ASN			54.764		50.005		36.25
496	CA	ASN			54.035		49.374		38.32
497	CB	ASN			55.074		48.740		39.80
498	CG	ASN			55.870		47.607		36.97
499		ASN			55.321		46.582		35.65
500		ASN			57.139		47.847		37.21
501	C	ASN			53.281		50.440		38.05
502	0	ASN			53.058		50.288		37.79 38.03
503	N	ILE			52.996		51.586		36.57
504	CA	ILE			52.081		52.641		
505	CB	ILE			52.790		53.920		36.46 33.71
506 507	CG1 CD1	ILE ILE			53.903 53.464		53.672 53.483		35.15
508	CG2	ILE			51.92		54.965		31.06
509	CGZ	ILE			50.979		52.797		38.05
510	0	ILE			51.256		52.869		35.21
511	N	ILE			49.724		52.661		37.36

FIGURE 3J

512 CA ILE A 676 48.617 41.868 52.857 1.00 37.03 513 CEI ILE A 676 47.229 41.162 52.874 1.00 37.73 515 CD1 ILE A 676 46.828 39.276 50.877 1.00 38.59 516 CG2 ILE A 676 46.105 42.067 53.361 1.00 39.38 517 C ILE A 676 48.978 42.142 55.242 1.00 35.26 518 O ILE A 676 48.978 42.142 55.242 1.00 32.27 519 N ARG A 677 48.683 43.918 54.025 1.00 34.27 520 CA ARG A 677 49.949 46.075 54.510 1.00 36.19 521 CB ARG A 677 49.9494 46.075 54.510 1.00 37.75 522 CR ARG A 677 49.9536 47.178 55.590 1.00 47.74 <t< th=""><th>A</th><th>В</th><th>С</th><th>D</th><th>E</th><th>F</th><th>G</th><th>Н</th><th>I</th><th>J</th></t<>	A	В	С	D	E	F	G	Н	I	J
513 CB ILE A 676 47.229 41.162 52.874 1.00 37.73 514 CCI ILE A 676 46.734 40.942 51.432 1.00 41.75 515 CDI ILE A 676 46.828 39.276 50.807 1.00 38.59 516 CG2 ILE A 676 48.796 42.654 54.162 1.00 39.38 517 C ILE A 676 48.978 42.142 55.242 1.00 32.27 519 N ARG A 677 48.683 43.918 54.025 1.00 32.27 520 CA ARG A 677 48.683 43.918 54.025 1.00 36.18 521 CB ARG A 677 49.536 47.178 55.599 1.00 41.64 522 CG ARG A 677 50.506 48.285 55.299 1.00 41.64 524 NE ARG A 677 49.995 49.516 53.246 1.00 51.85	512	CA	TLE	A	676	48.617	41.868	52.857	1.00	37.03
514 CG1 ILE A 676 46.734 40.942 51.432 1.00 41.75 515 CG2 ILE A 676 46.828 39.276 50.877 1.00 38.58 516 CG2 ILE A 676 48.105 42.654 54.162 1.00 35.26 518 O ILE A 676 48.978 42.142 55.242 1.00 32.27 519 N ARG A 677 48.683 43.918 54.025 1.00 34.27 520 CA ARG A 677 49.494 46.075 55.101 1.00 36.61 521 CB ARG A 677 49.536 47.178 55.599 1.00 41.64 522 CG ARG A 677 49.536 47.178 55.599 1.00 41.64 523 CD ARG A 677 49.825 49.350 54.572 1.00 53.55 525 CZ ARG A 677 49.095 50.568 52.734 1.00 55.75										
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518 O ILE A 676 48.978 42.142 55.242 1.00 32.27 519 N ARG A 677 48.683 43.918 54.252 1.00 34.27 520 CA ARG A 677 49.494 46.075 54.510 1.00 36.64 522 CG ARG A 677 49.494 46.075 54.510 1.00 36.64 523 CD ARG A 677 49.536 47.178 55.599 1.00 41.64 523 CD ARG A 677 49.825 49.350 54.572 1.00 53.55 525 CZ ARG A 677 49.825 49.350 54.572 1.00 53.55 526 NH1 ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 47.670 45.163 55.346 1.00 35.14 529 O ARG A 677 47.670 45.035 59.287 1.00 37.56 <tr< td=""><td></td><td>С</td><td>ILE</td><td>Α</td><td>676</td><td>48.796</td><td>42.654</td><td>54.162</td><td>1.00</td><td>35.26</td></tr<>		С	ILE	Α	676	48.796	42.654	54.162	1.00	35.26
520 CA ARG A 677 48.910 44.789 55.101 1.00 36.19 521 CB ARG A 677 49.494 46.075 54.510 1.00 36.64 522 CG ARG A 677 49.536 47.178 55.599 1.00 47.74 524 NE ARG A 677 49.825 49.350 54.572 1.00 53.55 525 CZ ARG A 677 49.795 49.516 53.246 1.00 54.93 526 NH1 ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 47.670 45.163 55.876 1.00 37.56 530 N LEU A 678 47.670 44.907 57.161 1.00 36.98 531 CA LEU A 678 46.577 45.306 58.012 1.00 37.75 532 CB LEU A 678 4		0	ILE	Α	676	48.978	42.142	55.242	1.00	32.27
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522 CG ARG A 677 50.536 47.178 55.599 1.00 41.64 523 CD ARG A 677 50.506 48.285 55.229 1.00 47.74 524 NE ARG A 677 49.795 49.516 53.246 1.00 61.80 526 NH1 ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 46.723 45.624 55.334 1.00 37.56 530 N LEU A 678 46.577 45.306 58.012 1.00 37.75 531 CA LEU A 678 46.637 45.306 58.012 1.00 37.75 532 CB LEU A 678 45.564 45.900 59.028 1.00 37.75 532 CB	520	CA	ARG	Α	677	48.910	44.789	55.101	1.00	36.19
523 CD ARG A 677 49.825 49.350 54.572 1.00 47.74 524 NE ARG A 677 49.825 49.350 54.572 1.00 53.55 526 NH1 ARG A 677 49.795 49.516 53.246 1.00 54.93 527 NH2 ARG A 677 49.096 50.568 52.734 1.00 35.75 528 C ARG A 677 47.670 45.163 55.876 1.00 37.16 529 O ARG A 677 46.723 45.624 55.334 1.00 37.55 530 N LEU A 678 46.577 45.306 58.012 1.00 37.75 531 CA LEU A 678 46.564 44.533 59.287 1.00 37.75 532 CB LEU A 678 45.944 53.06 58.012 1.00 36.72 533 CD	521	CB	ARG	А	677	49.494	46.075	54.510	1.00	36.64
524 NE ARG A 677 49.825 49.350 54.572 1.00 53.55 525 CZ ARG A 677 49.795 49.516 53.246 1.00 51.89 526 NH1 ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 46.670 45.163 55.876 1.00 35.14 529 O ARG A 677 46.723 45.624 55.334 1.00 37.75 530 N LEU A 678 46.670 44.907 57.161 1.00 37.75 531 CA LEU A 678 46.636 44.533 59.287 1.00 37.75 532 CB LEU A 678 44.636 44.533 59.287 1.00 37.75 534 CD1 LEU A 678 44.590	522	CG	ARG	А	677	49.536	47.178	55.599	1.00	41.64
525 CZ ARG A 677 50.425 48.610 52.436 1.00 54.93 527 NH2 ARG A 677 50.425 48.610 52.436 1.00 54.93 528 C ARG A 677 47.670 45.163 55.876 1.00 37.56 529 O ARG A 677 46.723 45.624 55.334 1.00 37.56 530 N LEU A 678 47.670 44.907 57.161 1.00 37.75 532 CB LEU A 678 46.636 44.533 59.287 1.00 37.75 532 CB LEU A 678 46.636 44.533 59.287 1.00 37.75 533 CG LEU A 678 44.186 44.629 59.808 1.00 40.66 535 CD2 LEU A 678 46.799	523	CD	ARG	Α	677	50.506	48.285	55.229	1.00	47.74
526 NH1 ARG A 677 50.425 48.610 52.436 1.00 54.93 527 NH2 ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 47.670 45.624 55.334 1.00 37.56 530 N LEU A 678 47.670 44.907 57.161 1.00 36.98 531 CA LEU A 678 46.636 44.533 59.287 1.00 37.15 532 CB LEU A 678 46.636 44.533 59.287 1.00 37.13 533 CG LEU A 678 45.644 45.003 60.367 1.00 38.89 534 CD1 A 678 44.590 59.808 1.00 36.72 536 CD LEU A 678 45.590 46.739 58.328	524	NE	ARG	Α	677	49.825	49.350	54.572	1.00	53.55
527 NH2 ARG A 677 49.096 50.568 52.734 1.00 55.75 528 C ARG A 677 47.670 45.163 55.876 1.00 35.14 529 O ARG A 677 46.723 45.624 55.334 1.00 37.56 530 N LEU A 678 47.670 44.907 57.161 1.00 36.95 531 CA LEU A 678 46.636 44.533 59.287 1.00 37.75 532 CB LEU A 678 46.636 44.533 59.287 1.00 37.13 534 CD1 LEU A 678 45.644 45.003 60.367 1.00 36.72 535 CD2 LEU A 678 45.909 44.223 61.548 1.00 36.735 537 O LEU A 678 47.505 47.253 58.861 1.00 36.755 538 CA	525	CZ	ARG	А	677	49.795	49.516	53.246		
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547 N GLY A 680 44.383 47.987 60.317 1.00 43.57 548 CA GLY A 680 43.778 48.130 61.635 1.00 43.39 549 C GLY A 680 42.428 47.436 61.718 1.00 43.49 550 O GLY A 680 41.870 46.994 60.730 1.00 43.61 551 N VAL A 681 41.917 47.300 62.921 1.00 43.77 552 CA VAL A 681 40.638 46.712 63.148 1.00 45.21 553 CB VAL A 681 40.739 45.577 64.095 1.00 44.87 554 CG1 VAL A 681 41.831 44.596 63.645 1.00 46.36 555 CG2 VAL A 681 39.714										
548 CA GLY A 680 43.778 48.130 61.635 1.00 43.39 549 C GLY A 680 42.428 47.436 61.718 1.00 43.49 550 O GLY A 680 41.870 46.994 60.730 1.00 43.61 551 N VAL A 681 41.917 47.300 62.921 1.00 43.77 552 CA VAL A 681 40.638 46.712 63.148 1.00 45.21 553 CB VAL A 681 40.739 45.577 64.095 1.00 44.87 554 CG1 VAL A 681 41.831 44.596 63.645 1.00 46.36 555 CG2 VAL A 681 41.163 46.141 65.458 1.00 48.19 556 C VAL A 681 39.714 47.667 63.826 1.00 47.24 557 O VAL A 681 40.146 48.697 64.420 1.00 47.24 <tr< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr<>										
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551 N VAL A 681 41.917 47.300 62.921 1.00 43.77 552 CA VAL A 681 40.638 46.712 63.148 1.00 45.21 553 CB VAL A 681 40.739 45.577 64.095 1.00 44.87 554 CG1 VAL A 681 41.831 44.596 63.645 1.00 46.36 555 CG2 VAL A 681 41.163 46.141 65.458 1.00 48.19 556 C VAL A 681 39.714 47.667 63.826 1.00 47.24 557 O VAL A 681 40.146 48.697 64.420 1.00 49.54 558 N ILE A 682 37.419 48.006 64.569 1.00 47.38 559 CA ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
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553 CB VAL A 681 40.739 45.577 64.095 1.00 44.87 554 CG1 VAL A 681 41.831 44.596 63.645 1.00 46.36 555 CG2 VAL A 681 41.163 46.141 65.458 1.00 47.24 557 O VAL A 681 39.714 47.667 63.826 1.00 47.24 558 N ILE A 681 40.146 48.697 64.420 1.00 49.54 558 N ILE A 682 38.444 47.292 63.827 1.00 47.38 559 CA ILE A 682 37.419 48.006 64.569 1.00 48.87 560 CB ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35 <		CA							1.00	45.21
554 CG1 VAL A 681 41.831 44.596 63.645 1.00 46.36 555 CG2 VAL A 681 41.163 46.141 65.458 1.00 48.19 556 C VAL A 681 39.714 47.667 63.826 1.00 47.24 557 O VAL A 681 40.146 48.697 64.420 1.00 49.54 558 N ILE A 682 38.444 47.292 63.827 1.00 47.38 559 CA ILE A 682 37.419 48.006 64.569 1.00 48.87 560 CB ILE A 682 36.375 48.569 63.710 1.00 48.42 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35						40.739	45.577	64.095	1.00	44.87
555 CG2 VAL A 681 41.163 46.141 65.458 1.00 48.19 556 C VAL A 681 39.714 47.667 63.826 1.00 47.24 557 O VAL A 681 40.146 48.697 64.420 1.00 49.54 558 N ILE A 682 38.444 47.292 63.827 1.00 47.38 559 CA ILE A 682 37.419 48.006 64.569 1.00 48.87 560 CB ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35						41.831	44.596		1.00	46.36
556 C VAL A 681 39.714 47.667 63.826 1.00 47.24 557 O VAL A 681 40.146 48.697 64.420 1.00 49.54 558 N ILE A 682 38.444 47.292 63.827 1.00 47.38 559 CA ILE A 682 37.419 48.006 64.569 1.00 48.87 560 CB ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35								65.458	1.00	48.19
558 N ILE A 682 38.444 47.292 63.827 1.00 47.38 559 CA ILE A 682 37.419 48.006 64.569 1.00 48.87 560 CB ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35		C	VAL	A	681	39.714	47.667	63.826	1.00	47.24
559 CA ILE A 682 37.419 48.006 64.569 1.00 48.87 560 CB ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35		0	VAL	A	681	40.146	48.697	64.420	1.00	49.54
560 CB ILE A 682 36.375 48.569 63.710 1.00 48.22 561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35	558	N	ILE	Α	682	38.444	47.292	63.827		
561 CG1 ILE A 682 36.958 49.768 62.995 1.00 48.43 562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35	559	CA	ILE	Α	682	37.419	48.006	64.569		
562 CD1 ILE A 682 35.994 50.531 62.288 1.00 44.35	560	CB	ILE	A	682	36.375	48.569	63.710		
	561	CG1	ILE	A	682	36.958	49.768			
563 CG2 ILE A 682 35.350 49.079 64.642 1.00 51.05	562	CD1	ILE	A	682	35.994				
	563	CG2	ILE	Α	682	35.350	49.079	64.642	1.00	51.05

FIGURE 3K

A	В	C	D	E		F	G	Н	I	J
564	С	TTD	7\	682	36	.787	46.983	65.439	1 00	49.28
				682		.073	46.091	64.927		47.34
565	O N	SER				.128	47.028	66.720		49.45
566	N							67.629		52.94
567	CA	SER				.611	46.043			
568	CB			683		.745	45.283	68.237		52.37
569	OG ~	SER				.501	46.148	69.035		57.12
570	C	SER				.865	46.665	68.798		55.66
571	0			683		.285	45.961	69.632		56.40
572	N			684		.893	47.987	68.884		57.01
573	CA	LYS				.286	48.589	70.046		57.46
574	CB			684		.154	49.729	70.595	1.00	
575	CG	LYS				.282	49.187	71.564	1.00	
576	CD	LYS				.630	49.925	71.446	1.00	
577	CE	LYS				.562	51.505	71.950		65.46
578	NZ			684		.871	52.366	71.881		62.96
579	С			684		.821	48.865	69.727		57.78
580	0			684		.999	48.795	70.580		58.15
581	N	TYR				.467	48.977	68.464		58.96
582	CA			685		.075	49.289	68.086	1.00	
583	CB			685		.994	50.682	67.473	1.00	
584	CG	TYR	Α	685		.713	51.794	68.195	1.00	
585	CD1	TYR	Α	685	32	.081	53.033	68.444		68.40
586	CE1	TYR	Α	685	32	.793	54.105	69.056	1.00	72.55
587	CZ	TYR	Α	685	34	.165	53.916	69.401	1.00	73.82
588	OH	TYR	Α	685	34	. 955	54.898	70.023		70.57
589	CE2	TYR	Α	685	34	.766	52.684	69.116	1.00	70.32
590	CD2	TYR	Α	685	34	.035	51.660	68.523	1.00	65.77
591	С	TYR	Α	685	31	.407	48.309	67.090	1.00	60.40
592	0	TYR	A	685	32	.026	47.310	66.713	1.00	61.88
593	N	LYS	Α	686	30	.162	48.569	66.649	1.00	59.90
594	CA	LYS	Α	686	29	.579	47.680	65.656	1.00	58.82
595	CB	LYS	Α	686	28	.498	46.716	66.024	1.00	59.93
596	CG	LYS	А	686	29	.096	45.424	66.530		59.37
597	CD	LYS	Α	686	29	.072	45.326	68.040	1.00	64.32
598	CE	LYS	Α	686	30	.146	46.244	68.676		67.97
599	NZ	LYS	А	686	30	.718	45.703	69.957	1.00	66.41
600	C	LYS	А	686	29	.658	47.859	64.242	1.00	59.00
601	0	LYS	Α	686	29	.403	48.925	63.673	1.00	61.49
602	N	PRO	Α	687	29	.432	46.717	63.735	1.00	56.91
603	CA	PRO	Α	687	30	.101	45.699	63.006	1.00	53.48
604	CB	PRO	Α	687	29	.846	46.015	61.546	1.00	55.46
605	CG	PRO	Α	687	28	.763	47.004	61.470	1.00	56.97
606	CD	PRO	Α	687	28	.593	47.506	62.796	1.00	57.11
607	C	PRO	Α	687	31	.572	45.851	63.404	1.00	50.95
608	0	PRO	Α	687	32	.164	46.919	63.374	1.00	49.51
609	N	MET				.169	44.784	63.861	1.00	48.57
610	CA	MET				.610	44.783	63.904		45.58
611	СВ	MET				.037	43.690	64.784	1.00	44.26
612	CG	MET					43.867	66.128		46.14
613	SD	MET					42.726	67.123		50.45
614	CE	MET						68.460		55.70
615	C	MET				.060	44.576	62.442		45.64
_										

FIGURE 3L

Α	В	С	D	E	F	G	H	I	J
	_		_		22 264	42 000	61 640	1 00	42.05
616	0			688	33.364		61.647		43.85
617	N			689	35.223		62.136		44.48
618	CA			689	35.872		60.853	1.00	
619	CB			689	35.682		60.344	1.00	
620	CG			689	34.291		60.319	1.00	
621	SD			689	33.939		59.192		42.01
622	CE			689	34.300		60.146		46.45
623	С			689	37.362		60.908		41.69
624	0			689	37.977		61.897		39.55
625	N			690	37.940		59.830		40.03
626	CA			690	39.410		59.726	1.00	
627	CB			690	39.650		59.574	1.00	
628	CG1			690	39.323		60.848		33.60
629	CD1			690	39.562		60.720		36.97
630	CG2	ILE	A	690	41.038		59.271		40.53
631	C	ILE	Α	690	39.644		58.495		38.31
632	0	ILE	Α	690	38.862		57.519	1.00	
633	N	ILE	А	691	40.509	45.952	58.568	1.00	39.22
634	CA	ILE	Α	691	40.764	46.894	57.444	1.00	36.53
635	CB	ILE	Α	691	40.907	48.317	57.943	1.00	37.55
636	CG1	ILE	А	691	39.876	48.734	59.047	1.00	39.31
637	CD1	ILE	Α	691	38.393	48.990	58.541	1.00	32.39
638	CG2	ILE	Α	691	40.907	49.256	56.831	1.00	37.29
639	C	ILE	Α	691	42.158	46.590	56.770	1.00	38.01
640	0	ILE	Α	691	43.218	46.620	57.463	1.00	38.01
641	N	THR	Α	692	42.182	46.381	55.445	1.00	37.20
642	CA	THR	Α	692	43.445	46.080	54.734	1.00	36.47
643	CB	THR	Α	692	43.566	44.593	54.387	1.00	35.20
644	OG1	THR	Α	692	42.564	44.283	53.451	1.00	35.83
645	CG2	THR	Α	692	43.156	43.824	55.543	1.00	30.57
646	C	THR	А	692	43.683	46.861	53.537	1.00	36.06
647	0	THR	Α	692	42.841	47.599	53.075	1.00	37.50
648	N	GLU	Α	693	44.893	46.762	53.018	1.00	36.84
649	CA	GLU	Α	693	45.200	47.581	51.862	1.00	34.75
650	CB	GLU	Α	693	46.688	47.414	51.456	1.00	34.83
651	CG	GLU	A	693	47.212	45.989	51.487	1.00	37.28
652	CD	GLU	Α	693	48.611	45.888	50.934	1.00	40.39
653	OE1	GLU	Α	693	49.308	44.958	51.275	1.00	45.33
654	OE2	GLU	Α	693	49.039	46.754	50.177	1.00	38.27
655	C	GLU	Α	693	44.262	47.082	50.823	1.00	35.09
656	0	GLU	A	693	43.970	45.920	50.773	1.00	36.98
657	N	TYR	Α	694	43.698	47.978	50.038	1.00	36.62
658	CA	TYR	Α	694	42.849	47.622	48.960	1.00	37.31
659	CB	TYR	A	694	42.179	48.887	48.452	1.00	37.54
660	CG	TYR	A	694	41.184	48.414	47.412	1.00	42.14
661	CD1	TYR	A	694	41.184	48.943	46.116	1.00	43.68
662	CE1	TYR			40.308	48.458	45.146	1.00	43.19
663	CZ	TYR	Α	694	39.456	47.373	45.442	1.00	43.99
664	OH	TYR			38.543		44.453	1.00	50.45
665		TYR			39.497		46.700	1.00	45.46
666		TYR					47.673		43.35
667	C			694	43.600		47.705		37.33

FIGURE 3M

А	В	C	D	E	F	G	Н	I	J
668	0	TYR	Α	694	44.550	47.410	47.236	1.00	36.42
669	N			695	43.211	45.693	47.297	1.00	36.44
670	CA			695	43.873	45.008	46.147	1.00	38.70
671	CB			695	44.266	43.583	46.553	1.00	36.76
672	CG			695	45.185	43.564	47.793	1.00	36.63
673	SD			695	46.870	44.267	47.620	1.00	38.01
674	CE			695	47.436	42.869	46.677	1.00	33.07
675	С			695	42.889	44.957	44.909	1.00	40.11
676	0			695	42.039	44.111	44.843	1.00	42.18
677	N	GLU	Α	696	43.005	45.883	43.975	1.00	40.26
678	CA	GLU	Α	696	42.088	46.032	42.896	1.00	41.93
679	CB	GLU	Α	696	42.712	46.973	41.893	1.00	43.18
680	CG			696	.42.480	48.440	42.115	1.00	48.76
681	CD			696	41.565	48.937	40.999	1.00	58.48
682	OE1	GLU	Α	696	40.566	48.194	40.663	1.00	63.90
683	OE2	GLU	Α	696	41.916	50.017	40.443	1.00	62.65
684	С	GLU	Α	696	41.889	44.764	42.103	1.00	41.93
685	O	GLU	Α	696	40.789	44.446	41.706	1.00	44.34
686	N	ASN	Α	697	42.922	43.979	41.880	1.00	39.85
687	CA	ASN	Α	697	42.618	42.947	40.921	1.00	38.87
688	CB	ASN	Α	697	43.808	42.705	39.966	1.00	38.40
689	CG	ASN	Α	697	43.812	43.672	38.784	1.00	40.20
690	OD1	ASN	Α	697	44.849	44.178	38.347	1.00	44.17
691	ND2	ASN	Α	697	42.558	43.959	38.269	1.00	45.86
692	C	ASN	Α	697	42.157	41.756	41.647	1.00	37.90
693	0	ASN	Α	697	41.992	40.689	41.026	1.00	39.69
694	N	GLY	Α	698	42.062	41.848	42.992		33.49
695	CA	GLY	Α	698	41.403	40.701	43.621	1.00	
696	C	GLY	А	698	42.204	39.491	43.680	1.00	29.77
697	0			698	43.383	39.592	43.682		29.55
698	N	ALA			41.559	38.342	43.701	1.00	
699	CA			699	42.186	37.154	43.998		29.38
700	CB	ALA			41.204	36.198	44.395		26.29
701	C	ALA			42.995	36.675	42.794		33.59
702	0			699	42.596	36.859	41.676		31.03
703	N	LEU		700	44.050	35.887	43.011	1.00	
704	CA	LEU		700	44.921	35.788	41.802		34.10
705	CB	LEU			46.407	35.560	42.179		32.00
706	CG	LEU			47.319	34.761	41.280		31.11
707		LEU		700	47.764	35.687	40.259		28.00
708	CD2	LEU			48.550	34.238	42.076		28.60
709	C	LEU			44.409	34.800	40.866		33.32
710	0	LEU			44.504	35.041	39.691		33.33
711	N	ASP			43.814	33.697	41.348		34.11
712	CA	ASP			43.402	32.617	40.406 41.064		35.12 33.80
713	CB	ASP			42.894	31.383			34.53
714 715	CG OD1	ASP ASP			41.715 41.531	31.594 32.676	41.891 42.421		30.09
716		ASP			40.923	30.670	42.421		37.42
717	C C	ASP			42.326	33.068	39.463		36.51
718	0	ASP			42.123	32.568			37.86
719	N	LYS			41.562	34.003	39.970		37.59
113	TA	טונ	1.7	, 02	41.702	24.003	32.310	1.00	55

FIGURE 3N

A	В	C	D	E	F	7	G	H	ı.	J
700	G.T.		_		40		24 520	20 110	1 00	26.66
720	CA			702	40.6		34.530	39.118		36.66
721	CB			702	39.3		34.752	39.976		39.28
722	CG	LYS			38.4		35.942	39.600	1.00	
723	CD			702	37.3		36.218	40.641	1.00	
724	CE			702	35.9		36.757	40.026	1.00	
725	NZ	LYS			35.1		35.733	39.227		67.51
726	C			702	40.8		35.646	38.132		35.74
727	0	LYS			40.2		35.681	37.082		37.89
728	N			703	41.5		36.665	38.605		33.13
729	CA			703	42.2		37.643	37.765		36.62
730	CB			703	43.3		38.312	38.567		34.46
731	CG			703	44.0		39.505	37.876		38.02
732	CD1	PHE			43.1		40.498	37.330		25.27
733	CE1	PHE			43.7		41.626	36.757		33.70
734	CZ	PHE		703	45.1		41.763	36.641		34.23
735	CE2	PHE		703	45.9		40.790	37.203		37.20
736	CD2	PHE		703	45.4		39.665	37.808		29.52
737	C	PHE		703	42.8		36.911	36.599		35.72
738	0	PHE			42.6		37.269	35.553		37.70
739	N	LEU			43.6		35.901	36.842	1.00	
740	CA	LEU			44.3		35.252	35.803	1.00	
741	CB	LEU			45.2		34.181	36.373		32.88
742	CG	LEU			46.4		34.749	37.087		36.11
743	CD1	LEU			47.3		33.579	37.374		37.94
744	CD2	LEU		704	47.1		36.016	36.306		37.86
745	С			704	43.4		34.649	34.912		36.85
746	0			70 4	43.7		34.499	33.721		35.55
747	N	ARG			42.2		34.267	35.435		38.22
748	CA	ARG			41.3		33.575	34.495		38.60
749	CB	ARG			40.2		32.784	35.157		37.82
750	CG	ARG			40.8		31.540	35.460		40.12
751	CD	ARG			39.8		30.555	35.686		40.84
752	NE ·	ARG		705	39.2		30.917	36.889		40.80
753	CZ	ARG			39.6		30.530	38.094		48.75
754	NH1	ARG			38.9		30.876	39.157		41.80
755	NH2	ARG			40.7		29.778	38.239	1.00	
756	C	ARG			40.6		34.528	33.555	1.00	
757	0	ARG			40.3		34.170	32.473		40.65
758	N	GLU			40.5		35.728	34.028		38.10
759	CA	GLU			39.9		36.744	33.282		40.40
760	CB	GLU			39.5		37.804	34.231		40.22
761	CG	GLU			38.2		37.363	34.881		50.24
762	CD	GLU			37.7		38.278	36.015		60.71
763	OE1	GLU			36.7		37.952	36.578		61.83
764	OE2	GLU			38.5		39.275	36.357	1.00	
765	C	GLU			40.9		37.385	32.278		38.37
766	0	GLU			40.4		38.051	31.411		40.23
767	N			707	42.1		37.278	32.465		37.18
768	CA	LYS			43.1		38.027	31.602		35.98
769	CB	LYS			44.0		38.856	32.502		36.31
770	CG	LYS			43.4		40.070	33.159		31.25
771	CD	LYS	A	707	42.5	37	40.850	32.178	1.00	41.00

FIGURE 3O

A	В	C	D	E		F	G	Н	I	J
772	CE	LYS	А	707		41.828	42.152	32.801	1.00	43.91
773	NZ	LYS				42.468	43.446	32.199	1.00	46.63
774	C	LYS				43.963	36.986	30.907	1.00	34.83
775	Ō			707	1	45.140	37.112	30.851	1.00	31.51
776	N	ASP				43.310	35.854	30.599	1.00	34.02
777	CA	ASP				43.961	34.687	30.142	1.00	34.42
778	CB	ASP				42.937	33.630	29.906	1.00	35.74
779	CG	ASP				43.549	32.340	29.318	1.00	37.91
780	OD1	ASP	A	708		44.713	32.065	29.373	1.00	46.66
781	OD2	ASP	Α	708		42.940	31.505	28.741	1.00	51.37
782	С	ASP		708		44.823	34.932	28.843	1.00	33.85
783	0	ASP	Α	708		44.332	35.563	27.880	1.00	33.03
784	N	GLY				46.076	34.438	28.842	1.00	32.14
785	CÁ	GLY				46.985	34.781	27.796	1.00	32.46
786	С	GLY	A	709		47.341	36.273	27.734	1.00	33.50
787	0	GLY	A	709		48.010	36.740	26.849	1.00	32.44
788	N	GLU	Α	710		47.011	37.043	28.715	1.00	33.77
789	CA	GLU	Α	710		47.365	38.445	28.521	1.00	35.02
790	CB	GLU	Α	710		46.198	39.448	28.823	1.00	34.74
791	CG	GLU	Α	710		44.870	39.054	28.228	1.00	33.49
792	CD	GLU	Α	710		43.843	40.107	28.521	1.00	41.03
793	OE1	GLU	Α	710		44.173	41.360	28.693	1.00	44.53
794	OE2	GLU	Α	710		42.704	39.661	28.521	1.00	38.77
795	\mathbf{C}_{\perp}	GLU	Α	710		48.602	39.017	29.221	1.00	36.64
796	0	GLU	Α	710		48.820	40.227	29.192	1.00	34.62
797	N	PHE	Α	711		49.403	38.185	29.832	1.00	37.09
798	CA	PHE	Α	711		50.510	38.792	30.525	1.00	37.88
799	CB	PHE				50.414	38.384	32.039	1.00	38.28
800	CG	PHE	А	711		49.322	39.225	32.812	1.00	38.60
801	CD1	PHE				48.302	38.610	33.509	1.00	38.93
802	CE1	PHE				47.359	39.316	34.196	1.00	36.81
803	CZ	PHE				47.377	40.696	34.129	1.00	
804	CE2	PHE				48.361	41.361	33.378	1.00	
805	CD2	PHE		711		49.320	40.609	32.722	1.00	36.32
806	C	PHE		711		51.731	38.237	29.795	1.00	38.37
807	0		A	711		51.653	37.191	29.189	1.00	38.38
808	N	SER		712		52.829	38.954	29.832	1.00	37.51
809	CA					54.054	38.463	29.318		37.68
810	CB	SER				55.019	39.640	29.207		33.41
811	OG	SER				55.482	39.865	30.488		38.72
812	C	SER				54.533	37.373			38.11
813	0	SER					37.370	31.560		36.94
814	N	VAL					36.430	29.853		36.56
815	CA	VAL					35.463	30.743		38.74
816	CB	VAL				56.860	34.555	29.902		40.25
817	CG1					57.880	33.741	30.734		40.91
818		VAL				55.973	33.661	29.047		46.85
819	C	VAL				56.820	36.172	31.891		38.93
820	0	VAL					35.653	33.003		38.80
821	N	LEU					37.366			38.01
822	CA	LEU						32.613		40.96
823	CB	LEU	A	/14		58.951	39.068	31.898	1.00	40.30

FIGURE 3P

A	В	C	D	E	F	G	Н	I	J
824	CG			714	60.120	39.781			45.88
825	CD1	LEU			61.094	38.833	33.052	1.00	
826	CD2	LEU	A	714	60.780	41.002	31.669	1.00	38.74
827	C	LEU	Α	714	57.168	38.638		1.00	40.29
828	0	LEU	А	714	57.505	38.570	34.844	1.00	44.01
829	N	GLN	A	715	55.998	39.165	33.341	1.00	39.22
830	CA	GLN	Α	715	55.001	39.613	34.321	1.00	36.85
831	CB	GLN	Α	715	53.868	40.332	33.636	1.00	38.50
832	CG	GLN	Α	715	54.218	41.672	33.012	1.00	29.96
833	CD	GLN	Α	715	53.075	42.067	32.167	1.00	28.87
834	OE1	GLN	Α	715	52.617	41.293	31.387	1.00	32.88
835	NE2	GLN	Α	715	52.490	43.193		1.00	33.61
836	C	GLN	Α	715	54.509	38.407	35.125	1.00	36.09
837	0	${\tt GLN}$	А	715	54.324	38.479	36.350	1.00	38.22
838	N	LEU	А	716	54.447	37.245	34.514	1.00	34.64
839	CA	LEU	Α	716	54.000	36.106	35.305	1.00	34.14
840	CB	LEU	Α	716	53.658	34.883	34.441	1.00	33.25
841	CG	LEU	Α	716	52.373	35.072	33.597	1.00	34.69
842	CD1	LEU	Α	716	52.021	33.922	32.684	1.00	40.42
843	CD2	LEU	Α	716	51.151	35.391	34.465	1.00	35.13
844	C	LEU	Α	716	55.008	35.742	36.325	1.00	36.34
845	0	LEU	Α	716	54.687	35.526	37.487	1.00	38.96
846	N	VAL	Α	717	56.247	35.640	35.901	1.00	35.71
847	CA	VAL	Α	717	57.282	35.173	36.716	1.00	33.91
848	CB	VAL	Α	717	58.571	35.031	35.931	1.00	35.17
849	CG1	VAL	Α	717	59.687	34.711	36.866	1.00	29.77
850	CG2	VAL	Α	717	58.367	33.983	34.852	1.00	38.75
851	C	VAL	Α	717	57.580	36.125	37.850	1.00	33.83
852	0	VAL	Α	717	57.880	35.699	38.947	1.00	31.28
853	N	GLY	A	718	57.534	37.416	37.555	1.00	31.97
854	CA	GLY	Α	718	57.503	38.426	38.592	1.00	35.27
855	С	GLY			56.292	38.282	39.565	1.00	36.66
856	0	GLY	A	718	56.491	38.537	40.791	1.00	39.82
857	N	MET	Α	719	55.089	37.891	39.114	1.00	35.07
858	CA	MET	Α	719	54.036	37.707	40.103	1.00	34.57
859	CB	MET	Α	719	52.605	37.454	39.502	1.00	34.98
860	CG			719	52.011	38.624		1.00	
861	SD	MET	A,	719	50.791	38.025	37.564	1.00	43.45
862	CE	MET	Α	719	50.085	39.579	36.958	1.00	37.28
863	C	MET	Α	719	54.549	36.568	40.960	1.00	34.85
864	0	MET	A	719	54.303	36.521	42.201	1.00	34.62
865	N	LEU			55.287	35.643	40.362	1.00	33.93
866	CA	LEU	Α	720	55.655	34.523	41.175	1.00	35.01
867	CB	LEU	А	720	56.042	33.265	40.370	1.00	34.91
868	CG	LEU	Α	720	54.807	32.554	39.778	1.00	
869	CD1	LEU			55.348	31.681	38.652	1.00	33.86
870	CD2	LEU			54.125	31.703	40.866		35.22
871	C	LEU		720	56.796	34.940	42.127		34.33
872	0	LEU			56.915	34.341	43.175		33.94
873	N	ARG		721	57.633	35.906	41.741		35.51
874	CA	ARG			58.698	36.200	42.637		37.80
875	CB	ARG	Α	721	59.987	36.862	42.044	1.00	38.19

FIGURE 3Q

A	В	С	D	E		F	G	Н	I	J
876	CG	ARG	Α	721	60.	314	38.329	42.432	1.00	43.45
877	CD	ARG				699	38.652	43.075		44.68
878	NE	ARG				671	39.968	43.738	1.00	46.01
879	CZ	ARG				115	40.223	45.005		47.92
880	NH1	ARG				690	39.297	45.760	1.00	42.62
881	NH2	ARG				011	41.426	45.507	1.00	42.77
882	С			721	58.	073	36.904	43.840	1.00	35.74
883	0	ARG	Α	721	58.	397	36.583	44.921	1.00	36.27
884	N	GLY	Α	722	57.	028	37.678	43.635	1.00	36.52
885	CA	GLY	А	722	56.	397	38.422	44.757	1.00	33.29
886	C	GLY	А	722	55.	861	37.381	45.691	1.00	32.31
887	0	GLY	Α	722	56.	178	37.333	46.854	1.00	33.65
888	N	ILE	А	723	54.	965	36.546	45.211	1.00	30.16
889	CA	ILE	А	723	54.	543	35.518	46.137	1.00	30.15
890	CB	ILE			53.	772	34.400	45.387	1.00	29.03
891	CG1	ILE	A	723		614	35.088	44.763	1.00	
892	CD1	ILE				890	34.311	43.667		22.43
893	CG2			723		270	33.347	46.367		23.88
894	C			723	, 55.		34.939	46.875		29.85
895	0	ILE				643	34.733	48.086	1.00	
896	N	ALA				673	34.526	46.105	1.00	30.46
897	CA	ALA				762	33.758	46.736	1.00	30.64
898	CB	ALA				778	33.564	45.694	1.00	32.41
899	C	ALA				469	34.553	47.912		29.69
900	0	ALA				762	34.063	49.021		26.55
901	N	ALA				746	35.770	47.606		27.76
902	CA	ALA				310	36.650	48.550	1.00	30.34
903	CB	ALA				330	38.044	47.843		29.68
904	C	ALA				500	36.648	49.943	1.00	32.46
905	0	ALA				049	36.269	51.069 49.778	1.00	32.65 31.30
906	N	GLY				186	36.806 36.858	50.888	1.00	
907 908	CA C	GLY GLY				280 416	35.599	51.565	1.00	
909	0	GLY				515	35.595	52.766	1.00	37.79
910	N	MET				508	34.533	50.825	1.00	33.96
911	CA			727		597	33.296	51.482	1.00	36.78
912	CB			727		397	32.063	50.534	1.00	38.17
913	CG					028	31.722	50.128		35.85
914	SD	MET				739	31.892	51.569		33.45
915	CE	MET				924	30.327			30.52
916	C			727			33.177			40.08
917	Ō	MET					32.402	52.994		40.52
918	N	LYS				049	33.876	51.607		41.82
919	CA	LYS				369	33.753	52.222		43.04
920	CB	LYS			61.		34.367	51.426		42.93
921	CG	LYS			62.		34.461	52.374		45.08
922	CD	LYS				269	34.813	51.788		48.13
923	CE	LYS				367	34.940	52.974		60.10
924	NZ	LYS			65.	965	33.765	53.965	1.00	59.07
925	C	LYS	Α	728	60.	220	34.506	53.629		43.72
926	0	LYS	Α	728	60.	732	34.080	54.703		42.16
927	N	TYR	A	729	59.	566	35.633	53.588	1.00	41.05

FIGURE 3R

A	В	С	D	E		F	(3]	H	I	J
928	CA	TYR	Α	729	59	.283	36.2	265	54.	861	1.00	40.26
929	CB	TYR				.511	37.4		54.			36.34
930	CG	TYR	Α	729	58	.276	38.2	219	55.	647	1.00	43.34
931	CD1	TYR	Α	729	59	.290	39.0	022	56.	234	1.00	41.12
932	CE1	TYR			58	.907	39.9	900	57.	404		41.14
933	CZ	TYR	A	729	57	.600	39.8		57.	863	1.00	
934	OH	TYR			56	.977	40.5	579	58.	883	1.00	40.30
935	CE2	TYR	Α	729	56	.672	38.9	976	57.	197	1.00	40.74
936	CD2	TYR	Α	729	56	.985	38.2	255	56.	187	1.00	36.09
937	C	TYR	Α	729	58	.534	35.3	355	55.	862	1.00	42.10
938	0	TYR	Α	729	58	.996	35.0	98	57.	035	1.00	41.89
939	N	LEU	Α	730	57	.379	34.8	814	55.	422	1.00	42.02
940	CA	LEU	Α	730	56	.704	33.9	992	56.	335	1.00	39.74
941	CB	LEU	Α	730	55	.411	33.4	422	55.	779	1.00	38.11
942	CG	LEU	Α	730	54	.356	34.5	521	55.	426	1.00	39.93
943	CD1	LEU	Α	730	53	.208	33.8	351	54.	731	1.00	30.48
944	CD2	LEU	A	730	53	.843	35.5	522	56.	628	1.00	36.84
945	C	LEU	Α	730	57	.615	32.9	961	56.	868	1.00	40.93
946	0	LEU	Α	730	57	.590	32.6	614	58.	097	1.00	44.06
947	N	ALA	А	731	58	.379	32.3	366	56.	000	1.00	41.66
948	CA	ALA	A	731	59	.128	31.2	219	56.4	482	1.00	43.27
949	CB	ALA	Α	731	59	.665	30.3	304	55.	365	1.00	42.98
950	C	ALA	Α	731	60	.252	31.6	695	57.	426	1.00	43.66
951	0	ALA	Α	731	60	.645	31.0	018	58.	306	1.00	44.04
952	N	ASN	Α	732	60	.709	32.8	385	57.	279	1.00	44.35
953	CA	ASN	А	732	61	.713	33.2	276	58.	220	1.00	46.81
954	CB	ASN	Α	732	62	.560	34.3	350	57.	600	1.00	43.35
955	CG	ASN	Α	732	63	.616	33.	729	56.	588	1.00	48.96
956	OD1	ASN	Α	732	63	.954	32.5	507	56.	609	1.00	49.17
957	ND2	ASN	Α	732	64	.077	34.5	565	55.	670	1.00	51.65
958	C	ASN	Α	732	61	.050	33.5	532	59.	645	1.00	47.03
959	0	ASN	Α	732	61	593	33.3	105	60.	645	1.00	47.94
960	N	MET	Α	733	59	.861	34.3	149	59.	686	1.00	47.68
961	CA	MET	Α	733	59	.083	34.3	350	60.	880		45.27
962	CB	MET			57	.872	35.2	218	60.			43.96
963	CG	MET				.018	36.6		60.			48.30
964	SD	MET				.136	37.6		61.			58.32
965	CE	MET				.421	37.3		62.			52.36
966	C	MET				.590	33.0		61.			45.93
967	0	MET				.762	32.9			179		46.67
968	N	ASN				.121	31.8		60.			46.78
969	CA	ASN				.546	30.6		61.			47.20
970	CB	ASN				.754	30.3		62.			50.07
971	CG	ASN				.243	30.0		63.			56.81
972		ASN				.886	30.6		64.			57.16
973		ASN				.803	29.0		62.			59.81
974	C	ASN				.069	30.4		61.			45.73
975	0	ASN				.373	29.7		61.			43.13
976	N	TYR				.542	31.0		60.			44.71
977	CA	TYR				.107	30.8		60.0			43.29
978	CB	TYR				.443	32.1		59.			42.22
979	CG	TYR	A	735	53	.029	32.0	009	59.	724	1.00	41.13

FIGURE 3S

A	В	С	D	E	F	G	Н	I	J
980	CD1	TYR	А	735	52.152	32.131	60.814	1.00	40.42
981	CE1	TYR	Α	735	50.811	32.085	60.664	1.00	47.06
982	CZ	TYR	Α	735	50.271	31.907	59.374	1.00	47.34
983	OH	TYR	Α	735	48.915	31.764	59.227	1.00	46.64
984	CE2	TYR	Α	735	51.155	31.732	58.239	1.00	47.89
985	CD2	TYR	A	735	52.528	31.829	58.447	1.00	42.90
986	С	TYR	Α	735	54.792	29.913	58.861	1.00	41.63
987	0	TYR	Α	735	55.164	30.186	57.742	1.00	42.29
988	N	VAL	Α	736	54.158	28.820	59.140	1.00	38.41
989	CA	VAL	A	736	53.937	27.923	58.084	1.00	39.18
990	CB	VAL	Α	736	53.963	26.643	58.559	1.00	38.60
991	CG1	VAL	Α	736	53.334	25.786	57.440	1.00	44.99
992	CG2	VAL	Α	736	55.465	26.273	59.020	1.00	41.99
993	C	VAL	Α	736	52.508	28.121	57.602	1.00	40.83
994	0	VAL	Α	736	51.554	27.827	58.342	1.00	37.18
995	N	HIS	Α	737	52.358	28.570	56.348	1.00	38.45
996	CA	HIS	А	737	51.076	29.014	55.969	1.00	38.83
997	CB	HIS	Α	737	51.218	29.539	54.599		40.55
998	CG	HIS	Α	737	50.007	30.193	54.135	1.00	
999		HIS			48.855	29.463		1.00	
1000	CE1	HIS	А	737	47.910	30.315	53.492		39.74
1001	NE2	HIS			48.385	31.563	53.591		33.63
1002		HIS			49.695	31.497	54.039		31.88
1003	C	HIS			49.993	28.008	55.933		41.07
1004	0	HIS			48.797	28.237	56.357		44.04
1005	N	ARG			50.376	26.934	55.306		41.15
1006	CA	ARG			49.618	25.687	55.197		40.70
1007	CB	ARG			48.940	25.402	56.513		42.80
1008	CG	ARG			49.697	24.932	57.725		45.84
1009	CD	ARG			48.687	24.798	58.849	1.00	
1010	NE	ARG			49.009	23.892	59.954		67.74
1011	CZ	ARG			48.085	23.420	60.827		72.67
1012	NH1	ARG			46.820		60.649	1.00	73.68
1013	NH2	ARG			48.410	22.631	61.865	1.00	72.81
1014	C	ARG			48.515	25.670 24.641	54.118	1.00	38.77 38.45
1015	O M	ARG ASP		738	47.921 48.177	26.788	53.870 53.516	1.00	
1016 1017	N CA	ASP			47.072		52.631		36.55
1017	CB	ASP			45.883	27.404	53.377		39.05
1019	CG	ASP		739	44.538	27.308	52.614		42.96
1020	OD1	ASP		739	43.754	28.312	52.665		43.61
1021		ASP		739	44.148	26.255	52.038		39.35
1022	C	ASP		739	47.535	27.617	51.504		36.75
1023	0	ASP		739	46.777	28.532	50.983	1.00	
1024	N	LEU		740	48.780	27.439	51.069	1.00	
1025	CA	LEU		740	49.061	28.504	50.134		33.57
1026	CB	LEU		740	50.481	28.864	50.075		33.24
1027	CG	LEU		740	50.940	29.335	48.750		31.68
1028	CD1	LEU		740	50.941	30.966	48.641		25.60
1029	CD2	LEU		740	52.323	28.912	48.706		23.37
1030	C	LEU			48.490	28.150	48.796		33.56
1031	0	LEU			48.501	26.963	48.357	1.00	31.12

FIGURE 3T

1032 N	A	В	С	D	E	F.	G	Н	I	J
1033	1032	N	ALA	A	741	47.907	29.154	48.172	1.00	32.21
1034								46.941	1.00	31.18
1036						45.926	27.914			
1036		С				46.846		46.143	1.00	29.34
1038 CA ALA A 742 46.506 31.125 44.116 1.00 30.53 1039 CB ALA A 742 46.415 30.932 42.505 1.00 29.25 1040 C ALA A 742 45.283 31.834 44.608 1.00 29.27 1041 O ALA A 742 45.243 31.003 44.528 1.00 31.53 1042 N ARG A 743 44.245 31.119 44.944 1.00 30.98 1044 CB ARG A 743 41.863 30.923 45.700 1.00 34.10 1046 CD ARG A 743 41.108 28.958 47.187 1.00 34.41 1047 NE ARG A 743 41.222 28.546 48.614 1.00 45.39 1049 NH1 ARG A 743 41.206 27.199 50.343 1.00 45.40 1050 NE2 ARG A 743 42.066 27.199 50.343 1.00 46.924		0				46.668	31.011	46.680	1.00	33.20
1039	1037	N	ALA	Α	742	46.670	29.881	44.843	1.00	30.74
1040	1038	CA	ALA	Α	742	46.506	31.125	44.116	1.00	30.53
1041 O ALA A 742 45.243 33.003 44.528 1.00 31.53 1042 N ARG A 743 44.245 31.119 44.944 1.00 30.98 1044 CB ARG A 743 41.863 30.923 45.700 1.00 34.10 1045 CG ARG A 743 41.108 28.958 47.187 1.00 34.41 1046 CD ARG A 743 41.108 28.958 47.187 1.00 34.44 1047 NE ARG A 743 41.222 28.546 48.614 1.00 45.39 1048 CZ ARG A 743 41.915 27.457 49.044 1.00 45.40 1050 NH2 ARG A 743 42.006 27.199 50.343 1.00 45.40 1051 C ARG A 743 42.567 33.390 47.192 1.00 35.27 1052 O ARG A 743 42.567 33.390 47.192 1.00 35.27 <td>1039</td> <td>CB</td> <td>ALA</td> <td>Α</td> <td>742</td> <td>46.415</td> <td>30.932</td> <td>42.505</td> <td>1.00</td> <td>29.25</td>	1039	CB	ALA	Α	742	46.415	30.932	42.505	1.00	29.25
1042 N ARG A 743 44.245 31.119 44.944 1.00 30.98 1043 CA ARG A 743 43.077 31.884 45.424 1.00 34.86 1045 CG ARG A 743 42.121 30.047 46.920 1.00 34.44 1046 CD ARG A 743 41.108 28.958 47.187 1.00 39.03 1047 NE ARG A 743 41.222 28.546 48.614 1.00 45.39 1049 NH1 ARG A 743 42.514 26.617 48.179 1.00 45.40 1050 NH2 ARG A 743 42.567 33.390 47.192 1.00 35.06 1051 C ARG A 743 42.567 33.390 47.192 1.00 35.06 1053 N ASN A 744 44.557 32.422 47.395 1.00 34.09 1055 CB </td <td>1040</td> <td>C</td> <td>ALA</td> <td>Α</td> <td>742</td> <td>45.285</td> <td>31.834</td> <td>44.608</td> <td>1.00</td> <td>29.77</td>	1040	C	ALA	Α	742	45.285	31.834	44.608	1.00	29.77
1043 CA ARG A 743	1041	0	ALA	Α	742	45.243	33.003	44.528	1.00	31.53
1044 CB ARG A 743 41.863 30.923 45.700 1.00 34.10 1045 CG ARG A 743 42.121 30.047 46.920 1.00 34.44 1047 NE ARG A 743 41.108 28.958 47.187 1.00 45.39 1048 CZ ARG A 743 41.915 27.457 49.044 1.00 45.40 1050 NH2 ARG A 743 42.514 26.617 48.179 1.00 45.40 1050 NH2 ARG A 743 42.006 27.199 50.343 1.00 37.01 1051 C ARG A 743 42.567 33.390 47.192 1.00 35.06 1053 N ASN A 744 44.557 32.422 47.395 1.00 34.06 1054 CA ASN A 744 44.501 33.215 48.540 1.00 39.21 1055 CB<	1042	N	ARG	Α	743	44.245	31.119	44.944	1.00	30.98
1045 CG ARG A 743 42.121 30.047 46.920 1.00 34.44 1046 CD ARG A 743 41.108 28.958 47.187 1.00 39.03 1048 CZ ARG A 743 41.222 28.546 48.614 1.00 45.39 1049 NH1 ARG A 743 42.006 27.199 50.343 1.00 47.01 1051 C ARG A 743 42.006 27.199 50.343 1.00 47.01 1051 C ARG A 743 42.567 33.390 47.192 1.00 35.06 1053 N ASN A 744 44.557 32.422 47.395 1.00 34.09 1054 CA ASN A 744 44.5131 32.369 49.740 1.00 33.38 1055 CB ASN A 744 44.5131 32.369 49.740 1.00 39.21 1057 OD1	1043	CA -	ARG	Α	743	43.077	31.884	45.424		
1046 CD ARG A 743 41.108 28.958 47.187 1.00 39.03 1047 NE ARG A 743 41.222 28.546 48.614 1.00 45.39 1048 CZ ARG A 743 41.915 27.457 49.044 1.00 48.15 1050 NH1 ARG A 743 42.006 27.199 50.343 1.00 47.01 1051 C ARG A 743 43.400 32.651 46.746 1.00 35.27 1052 O ARG A 743 42.567 33.390 47.192 1.00 35.06 1053 N ASN A 744 44.801 33.215 48.540 1.00 34.09 1054 CA ASN A 744 44.801 33.215 48.540 1.00 37.53 1055 CB ASN A 744 43.885 31.484 50.204 1.00 37.53 1055 CB <td>1044</td> <td>CB</td> <td>ARG</td> <td>Α</td> <td>743</td> <td>41.863</td> <td>30.923</td> <td>45.700</td> <td>1.00</td> <td>34.10</td>	1044	CB	ARG	Α	743	41.863	30.923	45.700	1.00	34.10
1047 NE ARG A 743 41.222 28.546 48.614 1.00 45.39 1048 CZ ARG A 743 41.915 27.457 49.044 1.00 48.15 1050 NH2 ARG A 743 42.006 27.199 50.343 1.00 47.01 1051 C ARG A 743 42.006 27.199 50.343 1.00 47.01 1052 O ARG A 743 42.567 33.390 47.192 1.00 35.06 1053 N ASN A 744 44.557 32.422 47.395 1.00 34.09 1054 CA ASN A 744 44.557 32.422 47.395 1.00 37.53 1056 CG ASN A 744 44.5131 32.369 49.740 1.00 37.53 1056 CG ASN A 744 42.750 31.939 50.226 1.00 42.62 1058 CD </td <td>1045</td> <td>CG</td> <td>ARG</td> <td>Α</td> <td>743</td> <td>42.121</td> <td>30.047</td> <td>46.920</td> <td>1.00</td> <td>34.44</td>	1045	CG	ARG	Α	743	42.121	30.047	46.920	1.00	34.44
1048 CZ ARG A 743 41.915 27.457 49.044 1.00 48.15 1049 NH1 ARG A 743 42.514 26.617 48.179 1.00 45.40 1051 C ARG A 743 42.006 27.199 50.343 1.00 47.01 1052 O ARG A 743 42.567 33.390 47.192 1.00 35.27 1053 N ASN A 744 44.557 32.422 47.395 1.00 34.09 1054 CA ASN A 744 44.801 33.215 48.540 1.00 37.53 1056 CB ASN A 744 45.131 32.369 49.740 1.00 37.53 1056 CB ASN A 744 45.131 32.369 49.740 1.00 37.53 1056 CB ASN A 744 45.131 32.369 49.740 1.00 34.75 1057 ODI </td <td>1046</td> <td>CD</td> <td>ARG</td> <td>Α</td> <td>743</td> <td>41.108</td> <td></td> <td>47.187</td> <td></td> <td></td>	1046	CD	ARG	Α	743	41.108		47.187		
1049 NH1 ARG A 743 42.514 26.617 48.179 1.00 45.40 1050 NH2 ARG A 743 42.006 27.199 50.343 1.00 47.01 1051 C ARG A 743 42.567 33.390 47.192 1.00 35.06 1053 N ASN A 744 44.557 32.422 47.395 1.00 34.09 1054 CA ASN A 744 44.801 33.215 48.540 1.00 33.38 1055 CB ASN A 744 45.131 32.369 49.740 1.00 37.53 1056 CG ASN A 744 42.750 31.939 50.226 1.00 42.62 1057 ODI ASN A 744 42.750 31.939 50.226 1.00 42.62 1058 ND2 ASN A 744 45.837	1047									
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1052 O ARG A 743										
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1082 C VAL A 747 46.354 42.728 43.243 1.00 35.15										
		0	VAL	A	747					36.61

FIGURE 3U

A	В	C	D	E	F	G	Н	I	J
1084	N			748	47.265	43.612	43.005		38.24
1085	CA			748	46.877	45.028	42.924		38.34
1086	CB			748	47.567	45.802	44.082		36.64
1087	CG			748	49.029	46.025	43.866		41.61
1088		ASN			49.862	46.322	44.892		43.62
1089	ND2			748	49.440	45.937	42.561		30.49
1090	C			748	47.108	45.643	41.577		39.45
1091	0			748	47.639	44.987	40.711		40.04
1092	N			749	46.695	46.895	41.373		42.73
1093	CA			749	46.786	47.496	40.099		46.89
1094	CB			749	46.385	48.978	40.082		48.87
1095	OG			749	45.668	49.315	41.225		54.36
1096	C			749	48.144	47.270	39.473		47.52
1097	0			749	48.120	47.006	38.275	1.00	
1098	N			750	49.269	47.369	40.208		45.78
1099	CA			750	50.564	47.075	39.586		45.35
1100	CB			750	51.653	47.880	40.233		46.42
1101	CG			750	51.353	49.378	40.146	1.00	
1102		ASN			50.799	49.871	39.111	1.00	
1103		ASN			51.556	50.090	41.283	1.00	
1104	C			750	50.867	45.596	39.508		45.29
1105	0			750	51.983	45.229	39.197		47.66
1106	N			751	49.900	44.715	39.759		43.51
1107	CA			751	50.329	43.316	39.610		41.03
1108	CB			751	50.906	43.089	38.217		38.31
1109	CG			751	50.061	43.748	37.120		41.64
1110		LEU			50.758	43.503	35.751		38.27
1111		LEU			48.627	43.252	36.999		28.14
1112	C			751	51.261	42.713	40.682		38.95
1113	0			751	51.616	41.503	40.614		39.08
1114	N			752	51.532	43.481	41.722		38.48
1115	CA			752	52.201	42.927	42.911		37.62
1116	CB			752	52.407	44.027	43.985		41.07
1117	CG1	VAL			52.935	43.433	45.248		31.93
1118	CG2	VAL			53.374	45.187	43.434		39.70
1119	C	VAL			51.212	41.969	43.535	1.00	36.23
1120	0	VAL			50.109	42.327	43.656		37.11
1121	N	CYS			51.624	40.762	43.833		33.42
1122	CA	CYS			50.883	39.701	44.373		32.01
1123	CB	CYS		753	51.362	38.393	43.688		27.84
1124	SG	CYS			50.701	38.335	42.039		33.28
1125	C	CYS			51.225	39.605	45.855		32.33
1126	0	CYS			52.398	39.547	46.172		32.32
1127	N	LYS			50.219	39.528	46.741		32.94
1128	CA	LYS			50.507	39.386	48.166		32.10
1129	CB	LYS			50.162	40.696	48.875		33.13
1130	CG	LYS			50.605	41.963	48.135		29.06
1131	CD	LYS			50.285	43.144	49.026		35.71
1132	CE	LYS			50.643	44.415	48.261		35.80
1133	NZ	LYS			51.568	45.193	49.061		43.38
1134	C	LYS			49.841	38.219	48.816		32.31
1135	0	LYS	A	/54	48.692	37.924	48.506	1.00	34.15

FIGURE 3V

A	В	C	D	E	F	G	H	I	J
			_						
1136	N			755	50.518	37.575	49.758		31.55
1137	CA			755	49.978	36.428	50.386		33.31
1138	CB			755	51.025	35.620	51.198		30.88
1139	CG1			755	50.350	34.441	51.795		32.21
1140	CG2			755	52.084	34.964	50.251		34.24
1141	C			755	48.926	37.022	51.377		35.40
1142	0			755	49.168	38.016	52.005		32.54
1143	N			756	47.774	36.361	51.457		38.43
1144	CA			756	46.644	36.872	52.159		43.72
1145	CB			756	45.634	37.437	51.159		44.86
1146	OG			756	44.645	38.014	52.000		54.93
1147	C			756	46.074	35.651	52.814		43.72
1148	0			756	46.719	34.651	52.765		43.99
1149	N			757	44.911	35.707	53.430		43.35
1150	CA			757	44.410	34.492	54.043		45.65
1151	CB			757	44.275	33.425	53.015		46.32
1152	CG			757	43.724	32.150	53.635		52.75
1153		ASP			44.124	30.984	53.230		56.00
1154		ASP			42.867	32.274	54.510		43.97
1155	C			757	45.196	33.850	55.204		46.33
1156	0			757	45.641	32.720	55.119		45.10
1157	N			758	45.277	34.549	56.314		47.63
1158	CA			758	46.037	34.089	57.464		49.68
1159	CB			758	46.847	35.258	58.006		44.29
1160	CG			758	47.817	35.731	57.094		42.30
1161		PHE			47.593	36.864	56.368		42.22
1162		PHE			48.598	37.322	55.442		39.71
1163	CZ			758	49.746	36.532	55.255		36.81
1164	CE2	PHE			49.877	35.352	55.943	1.00	
1165	CD2	PHE			48.975	34.983	56.849		40.00
1166	C			758	44.974	33.723	58.453		52.68
1167	0			758	44.200	34.528	58.838		57.15
1168	N	GLY			44.861	32.587	58.977		55.94
1169	CA	GLY			43.688	32.622	59.798		61.61
1170	C	GLY			43.267		60.339		65.29
1171	0	GLY			42.694	30.466	59.606		67.00
1172	N	ALA			43.669	31.122	61.603		68.87
1173	CA	ALA			43.342	30.071	62.553		70.34
1174	CB	ALA			42.221	30.592	63.474		72.37
1175	C	ALA			43.001	28.691	62.018		70.84
1176	0	ALA			43.734	27.741	62.273		72.10
1177	N	LYS			 38.912	22.109	55.182		61.96
1178	CA			778	39.123	23.434	54.474		62.02
1179	CB	LYS			39.109	24.631	55.464		61.52
1180	CG	LYS			38.190	25.744	55.100		65.24
1181	CD	LYS			36.788	25.579	55.739		72.35
1182	CE	LYS			35.799	26.577	55.111		76.05
1183	NZ	LYS			34.359	26.088	55.161		78.40
1184	C	LYS			40.461	23.466	53.662		59.65
1185	0	LYS			40.624	24.295			60.18
1186	N	ILE			41.456				56.99
1187	CA	ILE	A	779	42.634	22.716	53.087	1.00	54.46

FIGURE 3W

A	В	С	D	E	F	•	G	ŀ	Ŧ	I	J
1188	СВ	ILE	А	779	44.0	03 2	2.769	53.7	748	1.00	54.83
1189	CG1			779	44.1		3.930	54.7			56.87
1190	CD1			779	45.3		3.813	55.6		1.00	59.36
1191	CG2			779	45.0		2.969	52.6		1.00	51.91
1192	C			779	42.6		1.521	52.1		1.00	51.97
1193	0			779	42.6		0.418	52.5		1.00	49.38
1194	N	PRO		780	42.5	95 2	1.796	50.9	31	1.00	51.16
1195	CA	PRO	Α	780	42.5	09 2	0.747	49.9		1.00	50.51
1196	CB	PRO	A	780	42.3	43 2	1.559	48.6	551	1.00	51.35
1197	CG	PRO		780	43.2		2.689	48.9	38	1.00	51.32
1198	CD	PRO	A	780	42.7	32 2	3.136	50.3	882	1.00	49.94
1199	C	PRO	Α	780	43.7	49 1	9.936	49.7	777	1.00	49.64
1200	0	PRO	Α	780	44.9		0.334	49.7	770	1.00	49.57
1201	N	ILE	Α	781	43.4	59 1	8.672	49.6	554	1.00	50.09
1202	CA	ILE	Α	781	44.5	59 1	7.737	49.5	516	1.00	48.15
1203	CB	ILE	Α	781	43.9	70 1	6.376	49.2	235	1.00	48.98
1204	CG1	ILE	Α	781	43.1	.56 1	5.898	50.4	158	1.00	49.76
1205	CD1	ILE	Α	781	43.9	25 1	4.976	51.3	333	1.00	45.76
1206	CG2	ILE	Α	781	45.1	25 1	5.350	48.9	961	1.00	49.83
1207	C	ILE	Α	781	45.5	12 1	8.088	48.3	393	1.00	48.04
1208	0	ILE	Α	781	46.7	69 1	7.996	48.5	510	1.00	48.83
1209	N	ARG	Α	782	44.9		8.437	47.2	261	1.00	47.13
1210	CA	ARG	Α	782	45.8	02 1	8.586	46.0	83	1.00	45.63
1211	CB	ARG	Α	782	45.0	53 1	8.378	44.7	769	1.00	47.26
1212	CG	ARG	Α	782	44.0	23 1	9.394	44.3	396	1.00	44.31
1213	CD	ARG	Α	782	42.7	67 1	8.675	44.5	519	1.00	46.69
1214	NE	ARG	Α	782	42.1	41 1	8.708	43.2	274	1.00	56.04
1215	CZ	ARG	Α	782	41.4	62 1	7.713	42.7	740	1.00	56.10
1216	NH1	ARG	Α	782	40.9	77 1	7.877	41.5	06	1.00	56.62
1217	NH2	ARG	Α	782	41.3	06 1	6.594	43.4	100	1.00	52.79
1218	C	ARG	Α	782	46.6	63 1	9.814	45.9	54	1.00	44.90
1219	0	ARG	Α	782	47.3	49 1	9.960	44.9	28	1.00	43.83
1220	N	TRP	Α	783	46.6	18 2	0.701	46.9	956	1.00	42.72
1221	CA	TRP	А	783	47.5	51 2	1.768	46.9	95	1.00	39.98
1222	CB	TRP	А	783	46.8	68 2	3.004	47.4	12	1.00	37.95
1223	CG	TRP	A	783	46.4	79 2	3.843	46.3	300	1.00	35.96
1224	CD1	TRP	Α	783	47.1	44 2	4.953	45.8	329		37.75
1225	NE1	TRP	Α	783	46.4	42 2	5.528	44.7	784	1.00	33.74
1226	CE2	TRP	Α	783	45.2		4.838		89		27.42
1227	CD2	TRP	Α	783	45.2	34 2	3.816	45.6	30	1.00	27.27
1228	CE3	TRP	Α	783	44.1	58 2	2.941	45.6	65		39.26
1229	CZ3	TRP	Α	783	43.1	24 2	3.079	44.7	774	1.00	36.66
1230	CH2	TRP	Α	783	43.1	48 2	4.149	43.8	347	1.00	39.76
1231	CZ2	TRP			44.2		5.011	43.7			24.85
1232	C	TRP			48.5	80 2	1.312	48.0	36		38.70
1233	0	TRP			49.5		1.988	48.3			35.32
1234	N	THR			48.4		0.111	48.5	24		40.61
1235	CA	THR	Α	784	49.1		9.762	49.7	27		41.41
1236	CB		Α	784	48.2	21 1	9.287				43.19
1237	OG1	THR	Α	784	47.1	17 2	0.218			1.00	45.29
1238	CG2	THR	Α	784	48.9		9.287				34.46
1239	C	THR	A	784	50.1	98 1	8.707	49.5	43	1.00	42.11

FIGURE 3X

А	В	С	D	E	F	G	Н	I	J
1240	0	THR	Α	784	49.985	17.747	48.813	1.00	42.17
1241	N	ALA		785	51.327	18.906	50.196	1.00	42.96
1242	CA	ALA		785	52.418	17.963	50.141	1.00	44.73
1243	СВ	ALA		785	53.572	18.448	50.832	1.00	42.17
1244	С	ALA	Α	785	52.037	16.627	50.734	1.00	47.53
1245	0	ALA	Α	785	51.473	16.538	51.822	1.00	46.77
1246	N	PRO	Α	786	52.460	15.590	50.029	1.00	48.19
1247	CA	PRO	Α	786	52.143	14.221	50.417	1.00	50.36
1248	CB	PRO	Α	786	53.099	13.338	49.569	1.00	50.74
1249	CG	PRO	Α	786	53.928	14.299	48.752	1.00	49.25
1250	CD	PRO	Α	786	53.440	15.726	48.965	1.00	46.85
1251	C	PRO	Α	786	52.522	14.054	51.936	1.00	52.21
1252	0	PRO	Α	786	51.679	13.490	52.651	1.00	51.09
1253	N	GLU	Α	787	53.714	14.492	52.403	1.00	53.11
1254	CA	GLU	Α	787	53.970	14.318	53.884	1.00	55.40
1255	CB	GLU	Α	787	55.401	14.738	54.382	1.00	
1256	CG	GLU	Α	787	55.710	16.248	54.318	1.00	
1257	CD	GLU	Α	787	56.214	16.661	52.939	1.00	48.91
1258	OE1	GLU		787	56.021	15.847	52.033	1.00	44.65
1259	OE2	GLU		787	56.840	17.727	52.812	1.00	
1260	С	GLU		787	52.848	15.012	54.726	1.00	
1261	0	GLU		787	52.130	14.368	55.542	1.00	57.24
1262	N	ALA		788	52.713	16.318	54.544	1.00	54.35
1263	CA	ALA		788	51.644	16.988	55.186	1.00	54.04
1264	CB	ALA		788	51.446	18.323	54.578	1.00	53.00
1265	C	ALA		788	50.361	16.145	55.138	1.00	54.26
1266	0	ALA		788	49.670	16.086	56.112	1.00	54.80
1267	N	ILE		789	50.025	15.490	54.028	1.00	56.51
1268	CA	ILE		789	48.800	14.678	54.021	1.00	57.58
1269	CB	ILE		789	48.409	14.228	52.640	1.00	57.54 59.40
1270	CG1 CD1	ILE		789	47.712 47.797	15.332 15.085	51.828 50.262	1.00	54.27
1271 1272	CG2	ILE		789 789	47.309	13.160	52.772	1.00	60.10
1273	Ç	ILE		789	48.914	13.100	54.862	1.00	58.22
1274	ò	ILE		789	48.062	13.049	55.692	1.00	57.15
1275	N	SER		790	49.990	12.659	54.690	1.00	59.69
1276	CA	SER		790	49.932	11.382	55.316	1.00	61.39
1277	CB			790	50.549		54.444		61.41
1278	OG			790	51.936		54.315		61.74
1279	C			790	50.226		56.846		63.87
1280	Ō			790	49.485		57.593		64.38
1281	N	TYR			51.144		57.303	1.00	63.52
1282	CA	TYR			51.439		58.665	1.00	66.15
1283	CB	TYR			52.945		58.781	1.00	68.10
1284	CG	TYR			53.565		58.118		72.28
1285	CD1	TYR			54.150		56.854	1.00	
1286	CE1	TYR			54.755		56.241	1.00	
1287	CZ	TYR			54.770		56.900	1.00	
1288	ОН	TYR	Α	791	55.332		56.302	1.00	78.87
1289	CE2	TYR			54.210		58.176	1.00	
1290	CD2	TYR	Α	791	53.607	9.844	58.776	1.00	76.45
1291	С	TYR	A	791	50.974	13.612	59.238	1.00	66.97

FIGURE 3Y

A	В	С	D	Ε	F	G	Н	I	J
1292	0	TYR	A	791	51.182	13.912	60.434	1.00	66.84
1293	N	ARG			50.369	14.432	58.399	1.00	66.87
1294	CA	ARG			49.970	15.760	58.851	1.00	67.30
1295	CB	ARG	Α	792	48.869	15.753	59.940	1.00	68.23
1296	CG	ARG	Α	792	47.463	15.375	59.359	1.00	74.13
1297	CD	ARG	Α	792	46.869	14.030	59.780	1.00	82.23
1298	NE	ARG	A	792	45.886	14.125	60.886	1.00	89.59
1299	CZ	ARG	А	792	45.202	13.080	61.426	1.00	92.80
1300	NH1	ARG	Α	792	45.357	11.829	60.958	1.00	93.06
1301	NH2	ARG	А	792	44.347	13.285	62.440	1.00	92.12
1302	C	ARG	А	792	51.197	16.520	59.320	1.00	65.45
1303	0	ARG	Α	792	51.139	17.269	60.315	1.00	65.77
1304	N	ALA	А	793	52.306	16.318	58.611		63.00
1305	CA	ALA	A	793	53.519	17.103	58.883		61.10
1306	CB	ALA	A	793	54.867	16.228	58.776	1.00	60.85
1307	C	ALA			53.648	18.397	58.049		59.08
1308	0	ALA			54.293	18.378	56.975		58.44
1309	N			794	53.105	19.517	58.578		56.19
1310	CA	PHE			53.275	20.777	57.901		52.79
1311	CB			794	52.133	21.718	58.149		51.44
1312	CG			794	50.889	21.224	57.553		53.79
1313		PHE			50.266	20.110	58.096		50.68
1314		PHE			49.177	19.633	57:537	1.00	
1315	CZ	•		794	48.642	20.230	56.394		57.08
1316	CE2			794	49.263	21.310	55.814		48.15
1317	.CD2	PHE			50.350	21.819	56.416		51.41
1318	C	PHE			54.497	21.513	58.175		51.20 51.64
1319	O N	PHE			54.691 55.240	21.921 21.8 4 7	59.279 57.116		49.90
1320 1321	N CA	THR THR			56.318	22.788	57.254	1.00	
1321	CB	THR		•	57.644	22.788	57.445	1.00	
1323	OG1	THR			58.072	21.514	56.183	1.00	
1324	CG2	THR			57.447	20.906	58.372	1.00	
1325	C	THR			56.471	23.771	56.117		45.29
1326	0	THR			55.655	23.860	55.164		43.69
1327	N	SER			57.534	24.550	56.249		41.69
1328	CA	SER			57.818	25.476	55.208		41.82
1329	CB	SER			58.981	26.331	55.547	1.00	39.66
1330	OG	SER			58.361	27.301	56.341		44.72
1331	C	SER	Α	796	58.049	24.704	53.900	1.00	41.56
1332	0	SER	Α	796	57.696		52.871	1.00	41.54
1333	N	ALA	Α	797	58.524	23.473	53.999	1.00	40.13
1334	CA	ALA	Α	797	58.846	22.725	52.848	1.00	42.53
1335	CB	ALA	А	797	59.884	21.556	53.214	1.00	40.83
1336	C	ALA	A	797	57.521	22.169	52.280	1.00	42.33
1337	0	ALA	А	797	57.431	21.788	51.119	1.00	42.26
1338	N	SER			56.545	22.072	53.157		40.76
1339	CA	SER	A	798	55.253	21.629	52.760		40.11
1340	CB	SER			54.431	21.573	54.027		41.27
1341	OG	SER			53.766	20.389	53.989		46.94
1342	C	SER			54.772				39.12
1343	0	SER	А	798	54.056	22.735	51.062	1.00	39.97

FIGURE 3Z

A	В	С	D	E	F	G	Н	I	J
1344	N	ASP	Α	799	55.130	24.050	52.406	1.00	35.77
1345	CA			799	54.498	25.129	51.717		34.72
1346	СВ	ASP			54.780	26.453	52.486	1.00	33.36
1347	CG	ASP			53.791	26.726	53.664	1.00	34.25
1348		ASP			52.668	26.165	53.890	1.00	36.89
1349		ASP			54.068	27.559	54.447		37.78
1350	С			799	55.132	25.237	50.316	1.00	35.69
1351	0			799	54.570	25.868	49.348	1.00	37.88
1352	N			800	56.387	24.819	50.252	1.00	34.31
1353	CA			800	57.112	24.959	49.039	1.00	34.33
1354	СВ	VAL	Α	800	58.663	24.654	49.163	1.00	34.63
1355	CG1	VAL	Α	800	59.248	24.426	47.761	1.00	30.86
1356	CG2	VAL	Α	800	59.460	25.863	49.911	1.00	29.88
1357	C	VAL	Α	800	56.427	. 24.040	48.023	1.00	34.69
1358	0	VAL	Α	800	56.251	24.480	46.945	1.00	36.80
1359	N	TRP	Α	801	56.055	22.823	48.359	1.00	32.29
1360	CA	TRP	Α	801	55.170	22.045	47.475	1.00	34.84
1361	CB	ŤRP	Α	801	54.679	20.731	48.117	1.00	35.44
1362	CG	TRP	Α	801	53.843	19.907	47.285	1.00	33.44
1363	CD1	TRP	Α	801	52.561	20.102	46.984	1.00	32.49
1364	NE1	TRP	Α	801	52.070	19.046	46.260	1.00	32.97
1365	CE2	TRP	Α	801	53.073	18.136	46.097	1.00	33.72
1366	CD2	TRP	Α	801	54.183	18.623	46.756	1.00	34.03
1367	CE3	TRP	Α	801	55.320	17.800	46.841	1.00	38.46
1368	CZ3	TRP	Α	801	55.378	16.614	46.143	1.00	33.13
1369	CH2	TRP	Α	801	54.264	16.152	45.448		37.50
1370	CZ2	TRP	Α	801	53.088	16.888	45.430		42.25
1371	C	TRP	Α	801	53.951	22.760	47.036		34.91
1372	0	TRP	Α	801	53.531	22.621	45.934		38.09
1373	N	SER	Α	802	53.355	23.576	47.890		35.76
1374	CA	SER	Α	802	52.126	24.274	47.503	1.00	31.87
1375	CB			802	51.515	24.963	48.746		33.54
1376	OG			802	50.899	23.899	49.521		30.64
1377	C			802	52.429	25.304	46.557		31.93
1378	0			802	51.690	25.509	45.608		34.62
1379	N			803	53.536	26.007	46.779	1.00	
1380	CA			803	53.933	27.101	45.905	1.00	
1381	CB	PHE			55.219	27.653			29.35
1382	CG			803	55.817		45.639		32.84
1383		PHE			56.825		44.672		30.14
1384		PHE			57.313		43.909		28.45
1385	CZ			803	56.814		43.991		26.76
1386		PHE			55.846				30.61
1387		PHE			55.372	29.962	45.745		26.06
1388	C			803	54.263	26.610			30.18
1389	0	PHE			54.033	27.263			27.18
1390	N	GLY			54.777	25.406	44.421		32.24
1391	CA			804	54.953	24.865	43.033		33.84
1392	C			804	53.552				33.65
1393	0			804	53.373				31.75
1394	N			805		24.215			33.22
1395	CA	TĻĒ	A	805	51.181	24.192	42.565	1.00	33.26

FIGURE 3AA

A	В	C	D	E		F		G	H	I	J
1396	CB	ILE	А	805	50.	229	23	.528	43.503		33.65
1397	CG1			805	50.	811	22	.097	43.852		37.12
1398	CD1			805		975		.032	42.698		32.87
1399	CG2			805		823		.678	43.010		32.49
1400	С			805		696		.579	42.206		31.48
1401	0			805		103		.710	41.183		35.71
1402	N			806		019		.638	42.935		28.75
1403	CA			806		549		.991	42.575		25.41
1404	CB			806		961		.014	43.621		25.04
1405	CG1	VAL				941		.522	43.191		21.16
1406	CG2	VAL				157		.790	45.007		23.21
1407	С			806		341		.242	41.357		29.80
1408	0			806		912		.993	40.455		29.17
1409	N			807		538		.649	41.280		30.71
1410	CA			807		344		.966	40.092		31.44
1411	CB			807		785		.399	40.149		32.92
1412	CG			807		817		.157	41.066		31.62
1413	SD			807	-	439		.395	40.955		39.41
1414	CE			807		070		.142	40.672		45.05
1415	C			807		606		.493	38.830		31.38
1416	0			807		491		.212	37.876		33.09
1417	N			808		936		.352	38.875		31.98
1418	CA			808		347		.777	37.672		32.34
1419	CB			808		102		.315	38.067		33.08
1420	CG			808		501		.517	37.005		36.11
1421	CD1			808		163		.792	36.077		36.58
1422	NE1			808		257		.139	35.281		38.43
1423	CE2			808		005		.468	35.660		33.35
1424	CD2			808		123		.335	36.754 37.345		31.70 35.04
1425	CE3			808 808		968 744		.831	36.868		36.54
1426 1427	CZ3 CH2			808		638		.452 .571	35.743		38.94
1427	CZ2	TRP				760		.047	35.138		38.69
1429	C			808		064		.516	37.482		33.39
1430	0			808		612		.851	36.402		34.70
1431	N			809		457		.832	38.629		33.47
1432	CA			809		354		.714	38.567		30.38
1433	CB	GLU				563		.010	39.941		30.54
1434	CG	GLU				069		.930	40.924		28.60
1435	CD			809		429		.611	42.127		33.46
1436		GLU				269		.166	12.033		31.67
1437		GLU				163		.747	43.156		40.29
1438	C	GLU				610		.024	37.793		29.74
1439	0	GLU				798		.552	36.933		30.79
1440	N	VAL				656		.723	38.167		28.13
1441	CA	VAL				889		.000	37.520		26.64
1442	СВ	VAL		•		022		.716	38.242		26.67
1443		VAL				575		.853	37.310		22.89
1444		VAL				493		.103	39.725		27.59
1445	C	VAL				319		.755	35.999		28.59
1446	0	VAL				854		.404	35.114		24.03
1447	N	MET				055		.682	35.705	1.00	30.08

FIGURE 3AB

A	В	С	D	E	F	G	Н	I	J
1448	CA	MET	Α	811	51.499	29.612	34.339	1.00	31.44
1449	CB			811	52.744	28.783	34.201		35.04
1450	CG			811	54.001	29.305	35.125		31.45
1451	SD	MET			54.298	30.999	34.729	1.00	37.47
1452	CE	MET	Α	811	54.782	30.847	33.012	1.00	32.94
1453	C			811	50.347	29.060	33.524	1.00	34.61
1454	0	MET	Α	811	50.403	29.178	32.332	1.00	32.60
1455	N	THR	А	812	49.276	28.501	34.133	1.00	34.24
1456	CA	THR	Α	812	48.198	28.074	33.241	1.00	32.52
1457	CB	THR	Α	812	47.466	26.795	33.649	1.00	34.00
1458	OG1	THR	Α	812	47.141	26.876	35.053	1.00	32.67
1459	CG2	THR	Α	812	48.398	25.639	33.662	1.00	30.33
1460	С	THR	Α	812	47.135	29.096	33.341	1.00	31.91
1461	0	THR	Α	812	46.025	28.855	32.943	1.00	30.76
1462	N	TYR	Α	813	47.464	30.243	33.834		31.56
1463	CA			813	46.387	31.261	33.929		31.70
1464	CB			813	46.014	31.896	32.589		29.74
1465	CG			813	47.044	32.836	31.958		30.09
1466	CD1			813	48.104	32.376	31.114		28.85
1467	CE1	TYR			49.010	33.279	30.612		29.29
1468	CZ			813	48.842	34.593	30.910		29.69
1469	OH			813	49.541	35.655	30.375	1.00	
1470	CE2			813	47.824	35.015	31.708		31.05
1471	CD2	TYR			46.969	34.162	32.203		29.25
1472	C			813	45.134	30.738	34.656		30.85
1473	0 -	TYR			44.083	30.936	34.220		30.55
1474	N	GLY			45.270	30.031	35.753		33.19
1475	CA	GLY			44.090	29.747	36.568		35.27
1476	C			814	43.411	28.377	36.403		37.11 33.77
1477	O N	GLY			42.283 44.027	28.190 27.436	36.933 35.672		36.20
1478 1479	N CA			815 815	43.465	26.106	35.672		39.73
1479	CB			815	44.122	25.206	34.568		39.41
1481	CG			815	43.383	23.200	34.352		45.14
1482	CD	GLU			41.799	24.015	34.235		55.70
1483	OE1	GLU			41.019	24.346	35.224		48.24
1484		GLU			41.307	23.789	33.053		64.63
1485	C	GLU			43.505	25.458	37.133		40.38
1486	Ō	GLU			44.323				41.33
1487	N			816	42.636				41.29
1488	CA			816	42.531				42.57
1489	СВ	ARG			41.035	23.394	38.997		43.10
1490	CG	ARG			40.769	21.927	39.483		46.76
1491	CD	ARG	Α	816	39.291	21.462	39.802	1.00	54.39
1492	NE	ARG			39.376	20.573	40.974		59.04
1493	CZ	ARG			39.408	21.041	42.240	1.00	63.78
1494		ARG	Α	816	39.513	20.179	43.233	1.00	65.53
1495	NH2	ARG	Α	816	39.304	22.384	42.511	1.00	59.05
1496	C	ARG	A	816	43.464			1.00	41.97
1497	0	ARG	Α	816	43.398	21.857	37.823	1.00	42.38
1498	N			817	44.469	22.608			43.68
1499	CA	PRO	A	817	45.379	21.453	39.672	1.00	41.81

FIGURE 3AC

A	В	С	D	E	F	G	H	I	J
1500	СВ	PRO	А	817	46.156	21.699	40.929	1.00	41.78
1501	CG	PRO	Α	817	46.031	23.202	41.122	1.00	43.11
1502	CD	PRO	Α	817	44.749	23.678	40.560	1.00	40.66
1503	С			817	44.627	20.101	39.695	1.00	44.30
1504	0			817	43.467	19.877	40.271	1.00	45.86
1505	N			818	45.189	19.255	38.843	1.00	44.92
1506	CA			818	44.739	17.910	38.593		45.34
1507	СВ			818	44.740	17.159	39.884		43.91
1508	CG			818	46.093	17.345	40.535		42.86
1509	CD1	TYR			47.185	16.479	40.253	1.00	38.28
1510	CE1			818	48.459	16.660	40.852		37.76
1511	CZ			818	48.610	17.633	41.743		35.89
1512	OH			818	49.875	17.735	42.212		42.19
1513	CE2			818	47.577	18.531	42.049		33.24
1514	CD2			818	46.316	18.406	41.423		37.98
1515	C			818	43.336	17.995	38.033		47.01
1516	Ö			818	42.518	17.049	38.110		48.49
1517	N			819	43.005	19.164	37.505		47.05
1518	CA			819	41.701	19.253	36.867	1.00	
1519	СВ			819	41.740	18.432	35.528	1.00	
1520	CG			819	42.829	18.844	34.728	1.00	
1521	CD1			819	42.959	20.031	34.004		49.18
1522	NE1			819	44.228	20.119	33.441		43.97
1523	CE2			819	44.918	18.980	33.793		43.12
1524	CD2	TRP			44.087	18.187	34.609		47.93
1525		TRP			44.579	16.961	35.056		49.44
1526	CZ3	TRP			45.822	16.613	34.720		46.77
1527	CH2			819	46.585	17.392	33.912	1.00	
1528	CZ2			819	46.157	18.598	33.464		45.34
1529	C			819	40.560	18.743	37.751	1.00	
1530	Õ			819	40.418	19.134	38.920	1.00	
1531	N			820	39.757	17.855	37.170		53.15
1532	CA			820	38.614	17.241	37.872		54.37
1533	СВ			820	37.449	16.941	36.924		54.32
1534	CG			820	36.366	18.002	36.896	1.00	
1535	CD			820	36.972	19.390	36.838	1.00	
1536	OE1	GLU			36.651	20.232	37.703		63.58
1537		GLU			37.815		35.943		65.58
1538	C	GLU	Α	820	38.939	15.918	38.502	1.00	54.50
1539	0	GLU			38.032	15.090			56.40
1540	N	LEU			40.212	15.698	38.795		55.83
1541	CA	LEU			40.604	14.432	39.369		54.87
1542	CB	LEU			42.050	14.101	39.090		54.66
1543	CG	LEU			42.599	13.702	37.713		55.17
1544		LEU			44.138	14.023	37.650		59.74
1545		LEU			42.372	12.223	37.358		57.81
1546	C			821	40.311	14.322	40.862		55.57
1547	ō			821	40.184	15.328	41.610		52.91
1548	N	SER			40.208	13.053			55.96
1549	CA			822	39.800	12.777			56.75
1550	CB			822	39.132				57.57
1551	OG	SER			40.163	10.441	42.724		61.05
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FIGURE 3AD

A	В	С	D	E	F	G	Н	I	J
1552	Ċ	SER	Α	822	41.015	12.742	43.471	1.00	56.82
1553	0	SER	Α	822	42.111	12.351	43.029	1.00	55.43
1554	N	ASN	Α	823	40.752	13.039	44.733	1.00	57.38
1555	CA	ASN	Α	823	41.802	13.209	45.699	1.00	58.87
1556	CB	ASN	Α	823	41.242	13.615	47.073	1.00	58.15
1557	CG	ASN	Α	823	40.815	15.094	47.094	1.00	60.32
1558	OD1	ASN	Α	823	41.592	15.963	46.785	1.00	63.73
1559	ND2	ASN	A	823	39.582	15.363	47.432	1.00	61.31
1560	C	ASN	Α	823	42.513	11.941	45.660	1.00	59.12
1561	0	ASN	Α	823	43.753	11.872	45.759		60.64
1562	N	HIS			41.733	10.936	45.381	1.00	
1563	CA	HIS			42.274	9.608	45.413		60.00
1564	CB	HIS			41.115	8.627	45.445		60.99
1565	CG	HIS			41.565	7.246	45.256		67.03
1566		HIS			42.251	6.566	46.238		72.16
1567		HIS			42.594	5.370	45.772	1.00	
1568		HIS			42.189	5.271	44.513		75.73
1569		HIS			41.551	6.441	44.161	1.00	
1570	C	HIS			43.240	9.346	44.223	1.00	58.19 55.80
1571	O N	HIS		824	44.439 42.701	9.014 9.531	44.396 43.014		57.37
1572 1573	CA			825	43.514	9.516	41.785	1.00	
1574	CB			825	42.623	10.008	40.632	1.00	
1575	CG			825	41.881	8.907	39.881	1.00	
1576	CD			825	40.412	9.114	39.860	1.00	
1577	OE1	GLU			39.948	10.076	39.213	1.00	
1578	OE2	GLU			39.725	8.297	40.518		74.63
1579	C			825	44.764	10.399	42.063		54.94
1580	0			825	45.937	9.927	42.067	1.00	54.45
1581	N			826	44.529	11.648	42.467	1.00	53.85
1582	CA	VAL	Α	826	45.667	12.540	42.776	1.00	52.93
1583	CB	VAL	Α	826	45.208	13.870	43.319	1.00	51.81
1584	CG1	VAL	Α	826	46.447	14.871	43.452	1.00	52.68
1585	CG2	VAL	A	826	44.197	14.432	42.370	1.00	51.90
1586	C	VAL			46.759	11.943	43.687	1.00	
1587	0	VAL			47.967	11.917	43.378		53.40
1588	N	MET			46.363	11.447	44.821		53.41
1589	CA	MET			47.422				55.16
1590	CB	MET			47.018	10.882	47.148		55.87
1591	CG	MET			45.490	10.429	47.445		60.83
1592	SD	MET			44.615	10.847	49.114		65.49
1593	CE	MET			46.288	11.405	49.883		54.71
1594	C	MET			48.133	9.757	44.935 44.875		54.89 55.10
1595	O N	MET			49.401	9.704 8.861	44.875		55.10
1596 1597	N CA	ALA ALA			47.375 48.085	7.757	44.295		55.33
1597	CB	ALA			47.165	6.654	43.057	1.00	
1599	C	ALA			49.049	8.267	42.521	1.00	
1600	0	ALA			50.167	7.792	42.403	1.00	
1601	N	ALA			48.698	9.315	41.805		55.62
1602	CA	ALA			49.672	9.732	40.804		56.05
1603	СВ	ALA			49.103	10.831	39.898		56.37

FIGURE 3AE

A	В	С	D	E		F	G	Н	I	J
1604	С	ALA	Α	829		50.966	10.177	41.468	1.00	56.31
1605	Ō	ALA				52.116	9.756	41.108		56.19
1606	N			830		50.765	11.020	42.471	1.00	
1607	CA			830		51.891	11.651	43.112	1.00	
1608	СВ			830		51.446	12.581	44.293	1.00	57.35
1609	CG1	ILE	Α	830		50.835	13.861	43.719	1.00	56.71
1610	CD1	ILE	Α	830	•	51.574	14.320	42.496	1.00	47.37
1611	CG2	ILE	Α	830		52.641	12.975	45.149	1.00	52.92
1612	С	ILE	Α	830		52.767	10.611	43.637	1.00	58.16
1613	0	ILE	Α	830		54.003	10.637	43.431	1.00	58.31
1614	N	ASN	А	831		52.120	9.692	44.344	1.00	59.54
1615	CA	ASN	Α	831		52.883	8.672	45.016	1.00	60.79
1616	CB	ASN	А	831		52.033	7.966	46.046	1.00	62.19
1617	CG	ASN	Α	831		51.972	8.768	47.324		65.87
1618	OD1	ASN	Α	831		52.993	9.400	47.727	1.00	66.49
1619	ND2	ASN				50.781	8.826	47.934		68.01
1620	C	ASN				53.492	7.757	44.044	1.00	
1621	0	ASN				54.558	7.248	44.274		58.77
1622	N	ASP				52.860	7.609	42.896		59.28
1623	CA	ASP				53.530	6.790	41.905		60.01
1624	CB	ASP				52.494	6.118	41.014		60.55
1625	CG	ASP				52.076	4.698	41.576		66.55
1626		ASP				51.135	4.051	41.007	1.00	
1627		ASP				52.672	4.151	42.569		63.91
1628	C	ASP				54.697	7.455	41.121		59.37
1629	0	ASP				55.088	6.979	40.039		58.56
1630	N	GLY				55.293	8.525	41.664 40.850		58.64 57.55
1631	CA C	GLY GLY				56.220 55.529	9.303 9.892	39.615		57.72
1632 1633	0	GLY				55.730	9.408	38.503		61.73
1634	N	PHE				54.711	10.932	39.806	1.00	
1635	CA	PHE				53.992	11.588	38.713		52.71
1636	CB	PHE				52.692	10.831	38.438		52.86
1637	CG	PHE				52.758	9.760	37.377		55.68
1638	CD1	PHE				53.292	9.991	36.064		61.07
1639	CE1	PHE				53.276	8.953	35.053		58.90
1640	CZ	PHE				52.739	7.624	35.386	1.00	60.52
1641	CE2	PHE				52.202	7.400	36.702	1.00	56.50
1642		PHE				52.210	8.481	37.656	1.00	60.30
1643	C	PHE	Α	834		53.471	12.969	39.156	1.00	50.70
1644	0	PHE	Α	834		52.879	13.061	40.234	1.00	50.00
1645	N	ARG	Α	835		53.578	13.973	38.269	1.00	47.79
1646	CA	ARG	Α	835		53.278	15.397	38.529	1.00	47.62
1647	CB	ARG	Α	835		54.544	16.240	38.538	1.00	47.50
1648	CG	ARG	Α	835		55.739	15.796	39.492	1.00	48.70
1649	CD	ARG	Α	835		55.161	15.694	40.870	1.00	48.58
1650	NE	ARG	A	835		56.010	15.092	41.866		46.46
1651	CZ	ARG				55.778	13.923	42.395		45.45
1652		ARG				54.763	13.179	41.994		49.16
1653		ARG				56.575	13.478	43.301		47.75
1654	С	ARG				52.392	16.027			44.98
1655	0	ARG	А	835		52.160	15.415	36.403	1.00	46.68

FIGURE 3AF

A	В	С	D	E	F	G	Н	I	J
1656	N	LEU	Α	836	51.883	17.246	37.678	1.00	42.81
1657	CA			836	51.065	17.947	36.699	1.00	41.01
1658	CB			836	50.651	19.385	37.117	1.00	38.39
1659	CG	LEU	Α	836	49.702	19.386	38.291	1.00	40.70
1660	CD1	LEU	A	836	49.697	20.808	38.794	1.00	38.83
1661	CD2	LEU	Α	836	48.341	18.855	37.832	1.00	33.85
1662	C	LEU	Α	836	51.944	18.162	35.569	1.00	38.14
1663	0	LEU	Α	836	53.047	18.472	35.801	1.00	38.29
1664	N	PRO	Α	837	51.413	18.144	34.359	1.00	38.07
1665	CA	PRO	Α	837	52.214	18.316	33.157	1.00	36.29
1666	CB	PRO	Α	837	51.232	17.819	32.075	1.00	36.93
1667	CG	PRO	Α	837	49.907	18.505	32.492	1.00	35.54
1668	CD	PRO	Α	837	49.973	18.141	34.008	1.00	37.87
1669	C	PRO	Α	837	52.525	19.778	32.964		36.09
1670	0	PRO	Α	837	51.936	20.719	33.673		34.39
1671	N			838	53.406	20.032	32.013		34.01
1672	CA			838	53.894	21.359	31.903		35.98
1673	CB			838	55.120	21.485	30.963		36.64
1674	OG1	THR			55.395	22.892	30.765		39.83
1675	CG2	THR			54.736	21.181	29.545		38.71
1676	C			838	52.803	22.116	31.252		38.36
1677	0			838	52.197	21.670	30.274		39.45
1678	N			839	52.619	23.313	31.726		36.96
1679	CA			839	51.719	24.197	31.114		37.46
1680	CB			839	51.724	25.405	32.037		34.44
1681	CG			839	52.681	25.139	33.091		33.53
1682	CD			839	53.318	23.890	32.865		37.82
1683	C			839	52.285	24.602	29.749		38.53
1684	0			839	53.481	24.718	29.536		40.65
1685	N			840	51.382	24.872	28.840		40.11
1686	CA			840	51.632	25.423	27.501 26.953		42.06
1687	CB CG	MET MET		840	50.230 50.129	25.730 26.167	25.481		50.27
1688 1689	SD	MET			50.129	24.569	24.486		67.03
1690	CE	MET			51.027	25.324	23.049		53.52
1691	C	MET			52.554	26.728	27.544	1.00	
1692	0	MET			52.331	27.704	28.311		41.90
1693	N ·				53.600	26.738			39.46
1694	CA	ASP			54.541	27.802	26.665		38.39
1695	CB	ASP			53.847	28.967	26.104		36.97
1696	CG	ASP			53.255	28.676	24.629		40.53
1697		ASP			53.550	27.617	23.972		39.77
1698		ASP			52.445	29.466	24.066		36.62
1699	С	ASP			55.291	28.055	28.007		39.55
1700	0	ASP			55.749	29.129	28.326		41.50
1701	N	CYS			55.381	27.056	28.840		39.14
1702	CA	CYS			56.121	27.250	30.088	1.00	37.64
1703	CB	CYS			55.781	26.076	31.018		35.73
1704	SG	CYS			56.126	26.564	32.674	1.00	37.11
1705	C	CYS			57.616	27.200	29.840	1.00	36.94
1706	0	CYS			58.077	26.258	29.219	1.00	33.74
1707	N	PRO	A	843	58.352	28.267	30.217	1.00	37.65

FIGURE 3AG

A	В	С	D	E	F	G	H	I	J
1500	~=	220	_	0.4.2	FO 004	20 170	20 251.	1 00	34.75
1708	CA	PRO			59.804	28.178	30.251		
1709	CB			843	60.257	29.383	31.062		31.74
1710	CG	PRO			59.216	30.413	30.790		38.14
1711	CD	PRO			57.864	29.626	30.588		36.86
1712	C			843	60.258	26.981	30.973		34.58
1713	0	PRO			59.616	26.646	32.033		34.71
1714	N			844	61.364	26.414	30.439		30.44
1715	CA			844	61.947	25.239	30.957		32.01
1716	CB	SER			63.155	24.861	30.092		32.60
1717	OG -			844	63.939	23.905	30.735		32.71
1718	C			844	62.421	25.519	32.326		33.01
1719	0			844	62.327	24.669	33.152		34.58
1720	N			845	62.988	26.690	32.593		34.49
1721	CA			845	63.384	26.961	34.006		36.49
1722	CB			845	64.315	28.212	34.109		35.62
1723	C	ALA			62.124	27.066	34.982		34.14
1724	0	ALA			62.137	26.522	36.021		35.47
1725	N			846	60.992	27.590	34.558		33.95
1726	CA			846	59.787	27.597	35.457		31.95
1727	CB			846	58.778	28.539	34.866		33.95
1728	CG1			846	59.535	29.848	34.737		27.88
1729	CD1			846	59.817	30.375	36.417		26.15
1730	CG2			846	57.462	28.631	35.735		28.18
1731	C.			846	59.233	26.236	35.656		32.51
1732	0			846	59.054	25.847	36.786		31.68
1733	N			847	59.145	25.413	34.603		35.30
1734	CA			847	58.714	23.984	34.822		35.63
1735	CB			847	58.713	23.167	33.520		35.69
1736	CG			847	57.927	21.911	33.661		32.14
1737	CD1			847	58.477	20.696	33.310		27.77
1738	CE1			847	57.759	19.516	33.469		33.54
1739	CZ			847	56.522	19.509	34.064		31.43
1740	OH			847	55.943	18.320	34.231		40.26
1741	CE2	TYR			55.917	20.681	34.490		35.09
1742	CD2			847	56.645	21.928	34.253		32.81
1743	C			847	59.577	23.180	35.723	1.00	
1744	0			847	59.090	22.401	36.510	1.00	
1745	N	GLN			60.874	23.301	35.605		38.13
1746	CA	GLN			61.806	22.493	36.466		39.42
1747	CB			848	63.262	22.533	35.863		42.35
1748	CG	GLN			63.313	21.927	34.477		38.83
1749	CD	GLN			62.999	20.404	34.549		44.22
1750		GLN			62.228	19.877	33.736		48.28
1751		GLN			63.569	19.735	35.485		33.20
1752	C	GLN			61.821	22.902	37.950		36.31
1753	0	GLN			61.762	22.045	38.829		35.55
1754	N	LEU			61.847	24.194	38.200		37.37
1755	CA	LEU			61.716	24.680	39.552		38.40
1756	CB	LEU			61.552	26.151	39.507		37.22
1757	CG	LEU			61.237	26.406	40.933		36.60
1758		LEU			62.551	26.128	41.744		24.80
1759	CD2	LEU	A	849	60.902	27.913	40.922	1.00	33.30

FIGURE 3AH

A	В	С	D	E	F	G	Н	I	J
1760	С	LEU	A	849	60.521	24.099	40.250	1.00	39.79
1761	0	LEU	Α	849	60.540	23.685	41.468	1.00	43.91
1762	N			850	59.445	24.005	39.489	1.00	39.24
1763	CA	MET	Α	850	58.240	23.461	40.122	1.00	39.96
1764	CB	MET	А	850	56.904	23.372	39.299	1.00	40.95
1765	CG	MET	A	850	56.413	24.449	38.405	1.00	41.55
1766	SD	MET	Α	850	55.117	23.680	37.431	1.00	39.78
1767	CE	MET	Α	850	54.574	24.992	36.847	1.00	18.82
1768	C	MET	Α	850	58.422	22.040	40.423	1.00	37.52
1769	0	MET			57.783	21.573	41.370	1.00	38.53
1770	N	MET	Α	851	58.853	21.295	39.415		35.10
1771	CA	MET	А	851	59.106	19.877	39.608		37.40
1772	CB	MET			59.826	19.275	38.407		36.06
1773	CG	MET			58.932	19.130	37.200	1.00	
1774	SD	MET			57.537	18.184	37.411		43.74
1775	CE	MET			58.198	16.716	37.455		39.92
1776	C	MET			60.128	19.901	40.767		40.11
1777	0	MET			60.201	18.982	41.570		38.44
1778	N	GLN			60.894	20.980	40.908		39.68
1779	CA	GLN			61.720	20.958	42.059		42.72
1780	CB	GLN			62.918	21.868	41.882		41.86
1781	CG	GLN			63.758	21.298	40.778		52.95
1782	CD	GLN			65.096	22.010	40.537		62.78
1783	OE1				65.118	23.232	40.419		60.88
1784	NE2	GLN			66.203	21.229	40.419		69.19
1785	C	GLN			60.804	21.170	43.309		43.28
1786	0	GLN			60.916	20.491	44.309		43.36 43.67
1787	N .	CYS		853	59.818 59.046	22.048	43.242 44.454		41.63
1788 1789	CA CB	CYS			58.067	22.136 23.283	44.417		40.32
1790	SG	CYS			58.919	24.771	44.088	1.00	
1791	C	CYS			58.330	20.847	44.697		42.12
1792	0	CYS			57.934	20.608	45.832		42.69
1793	N	TRP			58.115	20.013	43.675		42.37
1794	CA	TRP			57.383	18.705	43.926		41.75
1795	CB	TRP			56.200	18.430	42.946		38.35
1796	CG	TRP			55.327	19.556	42.514		37.67
1797		TRP			54.684	20.557	43.330		35.33
1798		TRP			53.972	21.386	42.509		37.18
1799	CE2	TRP	Α	854	54.150	21.016	41.201	1.00	36.61
1800	CD2	TRP	Α	854	54.937	19.861	41.168	1.00	38.28
1801		TRP			55.238	19.302	39.913	1.00	35.92
1802	CZ3	TRP	Α	854	54.644	19.863	38.774	1.00	35.78
1803	CH2	TRP	Α	854	53.886	20.998	38.860	1.00	37.11
1804	CZ2	TRP	Α	854	53.642	21.597	40.055	1.00	36.88
1805	C	TRP	Α	854	58.249	17.379	44.163		43.48
1806	0	TRP	Α	854	57.788	16.232	43.928		40.95
1807	N	GLN	Α	855	59.470	17.495	44.694		46.45
1808	CA	GLN			60.141	16.215	45.033		47.97
1809	CB	GLN			61.562	16.399	45.421		49.14
1810	CG			855	62.300		44.563		53.78
1811	CD	GLN	A	855	63.599	16.874	43.944	1.00	57.56

FIGURE 3AI

A	В	C	D	E	F	G	Н	I	J
1812	OE1	GLN	Α	855	64.568	17.630	43.788	1.00	58.49
1813	NE2	GLN			63.597	15.574	43.550	1.00	
1814	C	GLN			59.503	15.583	46.185	1.00	
1815	0	GLN			59.135	16.279	47.106	1.00	
1816	N	GLN			59.417	14.251	46.193		50.70
1817	CA	GLN			58.760	13.603	47.270		51.94
1818	CB	GLN			58.589	12.110	47.008		52.72
1819	CG	GLN			57.987	11.341	48.190		56.53
1820	CD	GLN			56.902	10.378	47.730		67.51
1821	OE1	GLN			57.145	9.159	47.626	1.00	70.03
1822	NE2	GLN			55.687	10.921	47.421	1.00	70.24
1823	C	GLN			59.464	13.844	48.587	1.00	
1824	0	GLN			58.839	13.901	49.641		51.92
1825	N	GLU			60.776	13.978	48.540		53.47
1826	CA	GLU			61.455	14.329	49.763		52.94
1827	CB	GLU			62.751	13.574	49.888		55.76
1828	CG	GLU			63.760	13.655	48.776		62.73
1829	CD	GLU			64.555	12.357	48.808	1.00	75.13
1830	OE1	GLU			65.792	12.306	48.476	1.00	76.93
1831	OE2	GLU			63.876	11.369	49.244	1.00	80.58
1832	C	GLU			61.642	15.763	50.058	1.00	
1833	0			857	62.330	16.518	49.385		50.10
1834	N	ALA			61.062	16.140	51.162		51.40
1835	CA	ALA			60.918	17.553	51.501		51.01
1836	CB	ALA			60.376	17.634	52.879		51.91
1837	CP	ALA			62.236	18.232	51.481		52.16
1838	0	ALA			62.369	19.416	51.138		49.85
1839	N	ALA			63.210	17.476	51.130		52.64
1840	CA	ALA			64.489	18.044	52.311		51.38
1841	CB	ALA			65.270	17.114	53.176		52.83
1842	C	ALA			65.149	18.322	51.024		50.59
1843	0	ALA			66.033	19.188	50.921		52.09
1844	N	ARG			64.677	17.712	49.971		49.07
1845	CA	ARG			65.287	18.206	48.702		49.33
1846	CB	ARG			65.434	17.117	47.664		49.91
1847	CG	ARG			66.326	15.929	48.098	1.00	
1848	CD	ARG			66.767	14.950	46.979		67.86
1849	NE			860	67.897	15.592	46.310		79.99
1850	CZ	ARG			67.957	15.919	45.009		84.18
1851		ARG			69.035		44.538		86.30
1852	NH2	ARG			66.970	15.583	44.177		86.46
1853	C	ARG			64.642	19.423	48.073		47.17
1854	0	ARG			65.289	20.026	47.190		48.00
1855	N	ARG			63.390	19.778	48.428		43.32
1856	CA	ARG			62.722	20.886	47.710		42.70
1857	CB	ARG			61.279		48.284		43.25
1858	CG	ARG			60.375	19.925		1.00	38.41
1859	CD	ARG			58.992				33.61
1860	NE	ARG			58.563		48.956		39.84
1861	CZ	ARG			57.675		49.776		40.88
1862		ARG			57.041		50.621		47.18
1863		ARG			57.448	16.786	49.809		42.74

FIGURE 3AJ

A	В	С	D	E	F	G	Н	I	J
1864	C	ARG	Α	861	63.548	22.127	47.982	1.00	40.90
1865	0	ARG			64.151	22.197	49.048	1.00	45.17
1866	N			862	63.579	23.123	47.135	1.00	38.11
1867	CA			862	64.366	24.296	47.443	1.00	36.92
1868	СВ			862	64.173	25.174	46.248	1.00	37.49
1869	CG			862	62.978	24.528	45.479	1.00	34.16
1870	CD			862	62.827	23.232	45.881	1.00	36.86
1871	C	PRO	Α	862	63.565	24.973	48.494	1.00	40.68
1872	0	PRO	Α	862	62.378	24.679	48.675	1.00	38.28
1873	N	LYS	Α	863	64.195	25.936	49.155	1.00	43.10
1874	CA	LYS	Α	863	63.626	26.658	50.273	1.00	43.38
1875	CB	LYS	Α	863	64.689	26.934	51.402	1.00	44.69
1876	CG	LYS	Α	863	64.809	25.604	52.283	1.00	50.07
1877	CD	LYS	Α	863	65.801	25.501	53.459	1.00	60.38
1878	CE	LYS	A	863	65.260	26.211	54.856		67.58
1879	NZ	LYS	A	863	66.287	26.302	55.993		63.31
1880	С	LYS	Α	863	63.235	27.905	49.612		43.27
1881	0	LYS			63.753	28.275	48.476		45.68
1882	N			864	62.350	28.605	50.290		40.33
1883	CA			864	61.830	29.779	49.682		37.37
1884	CB			864	60.731	30.422	50.528		35.46
1885	CG			864	59.441	29.808	50.353		32.57
1886	CD1			864	58.869	29.099	51.365		34.21
1887	CE1			864	57.672	28.495	51.231		31.67
1888	CZ			864	56.964	28.622	49.961		31.72
1889	CE2	PHE			57.525	29.380	48.954		30.90
1890		PHE			58.743	29.927	49.129		37.14
1891	C			864	62.874	30.743	49.304	1.00	
1892	0			864	62.717	31.509	48.307		40.96
1893	N	ALA			63.875 64.964	30.905 31.837	50.126 49.712	1.00	38.95 40.21
1894 1895	CA CB	ALA ALA			66.009	31.987	50.851		40.74
1896	СВ	ALA			65.712	31.328	48.376		39.07
1897	0	ALA			66.186	32.133	47.578		40.17
1898	N	ASP			65.855	30.036	48.142	1.00	
1899	CA	ASP			66.437	29.657	46.850		41.20
1900	CB	ASP			66.592	28.205	46.710		42.25
1901	CG	ASP			67.356	27.563	47.886		46.38
1902		ASP			68.194		48.467	1.00	45.69
1903		ASP			67.164				46.52
1904	C	ASP			65.471	30.112	45.734		43.03
1905	0	ASP			65.895	30.862	44.786	1.00	43.71
1906	N			867	64.154	29.834	45.959		41.85
1907	CA	ILE	Α	867	63.161	30.097	44.945	1.00	39.25
1908	CB			867	61.738	29.686	45.429		40.79
1909	CG1			867	61.715	28.196	45.547	1.00	37.78
1910	CD1	ILE			60.587	27.644	46.393	1.00	31.95
1911	CG2			867	60.673	29.978	44.377	1.00	40.13
1912	C	ILE	Α	867	63.262	31.517	44.601	1.00	38.15
1913	0	ILE	А	867	63.383	31.839	43.478	1.00	34.00
1914	N	VAL	A	868	63.293	32.407	45.587	1.00	41.76
1915	CA	VAL	A	868	63.363	33.826	45.221	1.00	42.24

FIGURE 3AK

A	В	С	D	E	F	G	Н	I	J
1916	СВ	VAL	Α	868	63.468	34.646	46.495	1.00	43.37
1917	CG1			868	63.906	36.180	46.204		36.83
1918	CG2	VAL	Α	868	62.167	34.602	47.161	1.00	44.87
1919	С	VAL	Α	868	64.595	34.086	44.346	1.00	43.26
1920	0	VAL	Α	868	64.566	34.653	43.250	1.00	42.88
1921	N	SER	Α	869	65.709	33.593	44.819	1.00	43.82
1922	CA	SER	Α	869	66.947	33.788	44.034	1.00	45.81
1923	CB	SER	A	869	68.135	33.277	44.868	1.00	46.51
1924	OG	SER	А	869	69.256	32.973	44.081		55.81
1925	C			869	66.932	33.161	42.595		43.21
1926	0	SER	А	869	67.448	33.748	41.646		45.11
1927	N			870	66.309	32.041	42.410		40.48
1928	CA			870	66.341	31.421	41.081		41.53
1929	CB			870	65.721	30.078	41.130		40.21
1930	CG1			870	66.726	29.091	41.617		37.62
1931	CD1			870	65.913	27.844	42.278		34.59
1932	CG2			870	65.227	29.674	39.764	1.00	
1933	C			870	65.551	32.101	40.057		41.17
1934	0			870	65.629	31.841	38.862		45.96
1935	N			871	64.743	32.960	40.589		42.32
1936	CA			871	63.690	33.613	39.857		39.74
1937	CB			871 871	62.477	33.514 32.948	40.715		36.70 42.57
1938	CG				61.084		40.403		39.10
1939 1940	CD1 CD2	LEU LEU			61.128 60.155	31.584 32.800	39.753 41.647		33.43
1941	CDZ			871	64.073	35.062	39.677		40.56
1941	0			871	63.729	35.716	38.685		39.95
1943	N	ASP			64.858	35.710	40.655		43.30
1944	CA	ASP			65.641	36.754	40.333		45.25
1945	CB	ASP			66.270	37.416	41.537		44.64
1946	CG	ASP			65.296	38.054	42.370		50.39
1947		ASP			64.560	38.981	41.884	1.00	58.03
1948		ASP			65.222	37.729	43.584	1.00	59.66
1949	C	ASP	Α	872	66.617	36.467	39.147	1.00	42.59
1950	0	ASP	Α	872	66.673	37.301	38.244	1.00	40.36
1951	N	LYS	Α	873	67.123	35.244	39.030	1.00	43.85
1952	CA	LYS	A	873	68.158	35.043	37.946		46.85
1953	CB	LYS	Α	873	68.848	33.639	37.915	1.00	47.60
1954	CG	LYS			69.201	33.005	36.461		56.65
1955	CD			873 (32.494	36.301		64.86
1956	CE	LYS			71.327	31.621	37.470		72.42
1957	NZ	LYS			72.948	31.544	37.520	1.00	
1958	C	LYS			67.273	35.234	36.716	1.00	
1959	0	LYS			67.554	36.043	35.848		47.71
1960	N	LEU			66.177	34.496	36.670		44.00
1961	CA	LEU			65.345	34.413	35.523		41.76
1962	CB	LEU			64.257	33.510	35.950		42.33
1963	CG	LEU			64.335	32.030	35.627		43.61
1964		LEU			65.728	31.506	34.940		39.31
1965	CD2 C	LEU			63.820	31.183	36.838		40.93 41.73
1966	0	LEU		874 874	64.842 64.974	35.818 36.328	35.223 34.103		40.87
1967	J	TEO	А	0/4	04.9/4	30.328	34.103	1.00	±U.0/

FIGURE 3AL

A	В	С	D	E	F	G	Н	I	J
1968	N	TLE	А	875	64.356	36.539	36.219	1.00	41.36
1969	CA			875	63.986	37.926	35.895		41.48
1970	СВ			875	63.241	38.556	37.045	1.00	41.83
1971	CG1			875	61.848	37.830	37.313	1.00	
1972	CD1			875	61.307	38.014	38.707		42.11
1973	CG2			875	63.128	39.991	36.768		39.85
1974	C			875	65.128	38.822	35.369	1.00	43.50
1975	0			875	64.949	39.592	34.357	1.00	42.05
1976	N			876	66.305	38.724	36.005	1.00	43.68
1977	CA	ALA			67.460	39.526	35.543	1.00	47.29
1978	CB			876	68.686	39.705	36.633	1.00	45.33
1979	С			876	67.981	39.177	34.150	1.00	47.94
1980	0			876	68.349	40.096	33.381	1.00	49.38
1981	N			877	67.882	37.894	33.781	1.00	49.67
1982	CA			877	68.248	37.448	32.433	1.00	48.36
1983	CB			877	69.359	36.469	32.485	1.00	47.02
1984	С	ALA	Α	877	67.051	36.862	31.723	1.00	48.54
1985	0			877	66.995	35.680	31.364	1.00	48.87
1986	N	PRO	Α	878	66.165	37.720	31.333	1.00	48.50
1987	CA	PRO	Α	878	64.883	37.290	30.768	1.00	50.31
1988	CB	PRO	Α	878	64.248	38.609	30.314	1.00	49.52
1989	CG	PRO	Α	878	65.076	39.594	30.795	1.00	48.76
1990	CD	PRO	Α	878	66.399	39.140	31.199	1.00	47.09
1991	C	PRO	А	878	65.005	36.339	29.595	1.00	51.52
1992	0	PRO	А	878	64.080	35.558	29.329	1.00	52.11
1993	N	ASP	А	879	66.118	36.423	28.857	1.00	53.47
1994	CA	ASP	A	879	66.313	35.529	27.704	1.00	53.74
1995	CB	ASP	A	879	67.561	35.840	26.877	1.00	54.59
1996	CG	ASP	А	879	67.426	37.117	26.105	1.00	57.51
1997	OD1	ASP	Α	879	66.311	37.639	25.969	1.00	61.05
1998	OD2	ASP			68.385	37.705	25.618	1.00	63.66
1999	C			879	66.337	34.121	28.137	1.00	52.26
2000	0			879	66.064	33.243	27.320		52.16
2001	N			880	66.687	33.897	29.401	1.00	
2002	CA			880	66.494	32.578	30.001		49.70
2003	CB			880	66.869	32.588	31.504	1.00	52.27
2004	OG			880	65.870	33.209	32.357	1.00	50.20
2005	C			880	65.026	32.063	29.841		49.60
2006	0			880	64.796	30.895	29.773		49.66
2007	N			881	64.021	32.922	29.716		47.09
2008	CA			881	62.691	32.401	29.788		44.70
2009	CB			881	61.748	33.479	30.429		42.64
2010	CG			881	62.027	33.854	31.893		37.67
2011		LEU			61.053	35.053	32.335		46.29
2012		LEU			61.905	32.636	32.698		30.01
2013	C			881	62.230	31.982	28.406		46.11
2014	0			881	61.063	31.708	28.161		46.79
2015	N			882	63.166	31.996	27.480		46.05 44.09
2016	CA			882	62.872	31.829	26.034		44.09
2017	CB			882	63.999	32.408	25.172		50.65
2018	CG			882	63.822	33.855	24.808		
2019	CD	ГХS	A	882	64.615	34.299	23.548	1.00	57.85

FIGURE 3AM

A	B	C	D	E	F	G	Н	I	J
2020	CE	LYS	А	882	66.036	33.71	1 23.442		57.83
2021	NZ			882	66.063				
2022	C	LYS	A	882	62.712				
2023	0	LYS	Α	882	62.05				
2024	N			883	63.413				36.09
2025	CA			883	63.327				37.39
2026	CB			883	64.642				38.89
2027	OG1	THR			65.753				45.06
2028	CG2	THR			64.619				34.98
2029	C			883	62.325				37.20
2030	0			883	62.376				38.72
2031	N			884	61.468				
2032	CA			884	60.299				37.19
2033	CB			884	59.256				37.32
2034	CG			884	58.405				39.51
2035		LEU			59.168				40.46
2036		LEU			57.816				39.93
2037	C			884	60.536				37.90
2038	0			884	61.439				37.67
2039	N			885	59.766				40.12
2040	CA			885	59.817				43.23
2041	CB			885	59.092				40.83
2042	C			885	59.015				47.82
2043	0			885	58.130				48.49
2044	N			886	59.249				53.03
2045	CA			886	58.483				57.55
2046	CB			886	59.468				
2047	CG			886	59.80				66.52
2048		ASP			60.703				73.87 73.11
2049		ASP			59.214 57.476				58.65
2050 2051	C O			886 886	57.538				58.38
2051	N			887	56.513				62.53
2052	CA			887	55.793				63.20
2053	CB			887	56.793				63.87
2055	C			887	54.506				64.13
2056	0			887	53.476				64.69
4115		ATP			37.488				68.23
4116	PA	ATP			38.403				58.85
4117		ATP			39.539				63.08
4118		ATP			38.30				64.52
4119	PB			1000	37.326				65.46
4120		ATP			36.97				64.98
4121		ATP			38.372				
4122		ATP			36.030				
4123	PG			1000	36.102				64.66
4124		ATP			37.33				
4125		ATP			34.842				53.07
4126		ATP			36.34				55.85
4127		ATP			37.771				63.69
4128		ATP			36.564				51.19
4129		ATP			36.702				48.45
					· 				

FIGURE 3AN

4130	A	В	С	D	·E	F	G	Н	I	J
### ### ### ### ### ### ### ### ### ##	4130	04*	АТР	A 1	1000	36.838	39.812	48.897	1.00	48.02
A132 C2* ATP A1000 38.364 39.349 47.132 1.00 56.06 6133 O2* ATP A1000 37.709 39.459 45.885 1.00 53.71 4134 C3* ATP A1000 37.576 37.178 46.929 1.00 56.41 4135 O3* ATP A1000 38.870 40.760 48.977 1.00 46.97 4137 C8 ATP A1000 38.870 40.760 48.977 1.00 46.97 4137 C8 ATP A1000 40.236 40.299 50.155 1.00 45.86 4138 N7 ATP A1000 40.236 40.937 50.642 1.00 47.18 4139 C5 ATP A1000 40.553 41.923 49.802 1.00 45.85 4140 C6 ATP A1000 42.491 43.015 50.606 1.00 51.47 4142 C4 ATP A1000 42.491 43.015 50.606 1.00 51.47 4142 C4 ATP A1000 40.730 43.613 47.652 1.00 40.86 4144 C2 ATP A1000 40.730 43.613 47.652 1.00 40.86 4144 C2 ATP A1000 40.730 43.613 47.652 1.00 40.86 4145 N1 ATP A1000 41.527 43.736 48.735 1.00 37.92 4177 O HOH Y 301 34.209 7.517 100.111 1.00 42.77 4178 O HOH Y 303 36.987 20.304 84.823 1.00 48.24 4180 O HOH Y 305 38.693 6.951 84.781 1.00 33.40 4182 O HOH Y 305 38.693 6.951 84.781 1.00 33.40 4183 O HOH Y 306 43.619 28.688 43.907 1.00 36.33 4183 O HOH Y 307 33.5150 4.275 99.892 1.00 38.81 4184 O HOH Y 308 34.293 39.454 56.291 1.00 26.79 4185 O HOH Y 310 34.293 39.454 56.291 1.00 38.81 4184 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 4188 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 4188 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 4188 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 4189 O HOH Y 313 36.391 38.50 38										
A133 O2* ATP A1000 37.709 39.459 45.885 1.00 53.71 A134 C3* ATP A1000 37.962 38.092 47.863 1.00 56.21 A135 O3* ATP A1000 37.576 37.178 46.929 1.00 56.21 A136 N9 ATP A1000 38.870 40.760 48.977 1.00 48.97 A137 C8 ATP A1000 39.164 40.209 50.155 1.00 46.56 A138 N7 ATP A1000 40.236 40.937 50.642 1.00 47.18 A139 C5 ATP A1000 40.553 41.923 49.802 1.00 46.85 A140 C6 ATP A1000 41.495 42.912 49.749 1.00 45.05 A141 N6 ATP A1000 41.495 42.912 49.749 1.00 45.05 A141 N6 ATP A1000 39.721 41.807 48.758 1.00 44.98 A141 N3 ATP A1000 39.840 42.616 47.754 1.00 40.18 A143 N3 ATP A1000 41.527 43.613 47.652 1.00 40.86 A145 N1 ATP A1000 41.527 43.736 48.735 1.00 37.92 A177 O HOH Y 301 34.209 -7.517 100.111 1.00 42.77 A178 O HOH Y 303 36.987 20.304 84.823 1.00 48.24 A180 O HOH Y 303 36.987 20.304 84.823 1.00 36.33 A183 O HOH Y 305 38.693 6.951 84.781 1.00 30.63 A183 O HOH Y 308 43.693 6.951 84.781 1.00 36.33 A183 O HOH Y 308 34.293 39.454 56.291 1.00 26.79 A185 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 A188 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 A188 O HOH Y 311 52.468 18.101 40.466 1.00 34.94 A189 O HOH Y 311 50.636 25.308 51.909 1.00 26.94 A199 O HOH Y 315 38.314 43.464 44.478 1.00 33.90 A199 O HOH Y 316 58.592 38.679 69.488 1.00 42.08 A199 O HOH Y 317 34.711 38.223 45.323 1.00 38.90 A199 O HOH Y 318 51.004 34.502 28.290 1.00 35.17 A199 O HOH Y 316 58.592 38.679 69.458 1.00 42.08 A199 O HOH Y 317 34.711 38.223 45.323 1.00 38.90 A199 O HOH Y 318 51.004 34.502 28.290 1.00 38.97 A199 O HOH Y 323 50										
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FIGURE 3AO

A	В	С	D	E	F	G	Н	I	J
4213	0	нон	Y	338	27.063	12.328	81.741	1.00	49.23
4214	0	HOH	Y	339	43.495	-1.978	101.845	1.00	29.87
4215	0	HOH	Y	340	24.042	11.453	87.471	1.00	41.90
4216	0	HOH	Y	341	28.532	21.817	105.465	1.00	51.38
4217	0	HOH	Y	342	34.250	-2.816	87.557	1.00	40.16
4218	0	HOH	Y	343	61.321	37.753	51.409	1.00	42.73
4219	0	HOH	Y	344	36.839	-8.065	88.494	1.00	47.43
4220	0	HOH	Y	345	36.931	51.353	67.108	1.00	43.87
4221	0	HOH	Y	346	32.133	3.426	74.670		41.40
4222	0	HOH	Y	347	35.239	-3.830	103.044	1.00	32.29
4223	0	HOH	Y	348	29.414	4.943	100.046	1.00	41.59
4224	0	HOH	Y	349	24.239	20.789	98.495	1.00	55.55
4225	0	HOH	Y	350	. 56.249	24.229	27.459	1.00	35.32
4226	0	HOH	Y	351	42.039	36.733	27.828		31.77
4227	0	HOH	Y	352	49.598	14.602	89.944		39.22
4228	0	HOH	Y	353	53.086	45.810	55.315	1.00	46.66
4229	0	HOH	Y	354	56.134	28.666	55.481	1.00	37.89
4230	0	HOH	Y	355	63.607		51.318		45.92
4231	0	HOH	Y	356	47.007	-0.656	101.802		39.67
4232	0	HOH	Y	357	56.849	42.289			43.93
4233	0	HOH	Y	358	50.297	45.047	58.166		37.20
4234	0	HOH	Y	359	28.541	41.183			46.64
4235	0	HOH	Y	360	61.669	23.736			46.15
4236	0	HOH	Y	361	46.431	16.691	103.110		35.98
4237	0	HOH	Y	362	43.512	8.970	105.775		36.32
4238	0	HOH	Y	363	62.088	25.972	23.786		38.78
4239	0	НОН	Y	364	64.287	31.187			44.19
4240	0	нон			34.618	30.621			40.96
4241	0	нон			25.281	41.511			44.80
4242	0	HOH	Y	367	45.275	20.695	97.308	1.00	46.67

FIGURE 3AP

A	В	С	D	E	F	G	H	I	J
			_		61 500	1 805	0.00	1 00	== 60
2057	N			602	61.588	-1.705	97.096		75.62
2058	CA			602	61.031	-2.970	96.546	1.00	76.68
2059	CB	ALA		602	61.665	-3.292	95.199	1.00	76.47
2060	C			602	61.337	-4.080	97.519	1.00	77.44
2061	0	ALA		602	61.332	-5.311	97.156	1.00	75.75
2062	N			603	61.635	-3.605	98.744	1.00	77.75
2063	CA	LYS		603	62.173	-4.417	99.861	1.00	77.56
2064	CB	LYS		603	63.425	-3.748	100.411	1.00	78.96
2065	CG	LYS		603	63.212	-2.282	100.938	1.00	78.12
2066	CD	LYS		603	62.779	-2.211	102.422	1.00	78.99
2067	CE	LYS		603	63.952	-2.034	103.426	1.00	79.93
2068	NZ	LYS		603	64.536	-0.656	103.573	1.00	79.82
2069	C	LYS		603	61.103	-4.418		1.00	76.81
2070	0	LYS		603	61.315	-4.798	102.072	1.00	75.16
2071	N	PHE		604	59.938	-3.975	100.457	1.00	76.03
2072	CA	PHE		604	58.711	-3.929	101.207	1.00	74.92
2073	CB	PHE		604	58.102	-2.575	100.991	1.00	76.05
2074	CG	PHE		604	58.700	-1.538	101.857	1.00	78.39
2075	CD1			604	58.564	-1.631	103.231	1.00	79.39
2076	CE1			604	59.115	-0.671	104.059		84.10
2077	CZ	PHE		604	59.854	0.395	103.511		81.74
2078	CE2			604	60.017	0.474	102.144		82.47
2079	CD2				59.448	-0.503	101.312		81.05
2080	C			604	57.783	-5.006	100.707	1.00	73.54
2081	0			604	56.553	-4.941	100.826	1.00	73.46
2082	N			605	58.368	-6.069	100.190	1.00	71.71
2083	CA			605	57.496	-7.068	99.640		68.96
2084	CB			605	57.540	-6.922	98.163		68.75
2085	OG1			605	57.203	-8.191	97.632	1.00	71.34
2086	CG2			605	58.991	-6.774	97.722	1.00	71.15
2087	C			605	57.874	-8.494	99.969		65.74
2088	0			605	59.000	-8.868	99.864		66.65
2089	N			606	56.897	-9.294	100.339		61.47
2090	CA			606	57.083	-10.702	100.542		56.89
2091	CB			606	55.818	-11.150	101.234		58.04
2092	OG1	THR		606		-10.407	102.470		53.91
2093	CG2	THR		606	55.854	-12.662	101.579	1.00	56.07
2094	C	THR		606	57.153	-11.402	99.182		55.32
2095	0			606	56.376	-11.139	98.285		55.18
2096	N	GLU		607	58.053	-12.330	99.008		52.87
2097	CA			607	58.113	-13.077	97.771		48.83
2098	CB	GLU		607	59.550	-13.585	97.546	1.00	
2099	CG	GLU		607	59.720	-14.650	96.488		49.52
2100	CD	GLU	В	607	59.828	-14.069	95.132	1.00	53.13

FIGURE 3AQ

A	В	С	D	E	F	G	Н	I	J
2101	OE1	GLU	R	607	59.999	-12.782	95.021	1.00	47.52
2102	OE2	GLU		607	59.708	-14.931	94.179	1.00	
2103	C	GLU		607	57.128	-14.194	97.907	1.00	
2104	0			607	57.022	-14.795	98.940	1.00	
2105	N			608	56.391	-14.548	96.865	1.00	47.65
2106	CA			608	55.448	-15.608	97.148	1.00	47.68
2107	CB			608	54.064	-15.132	96.825	1.00	48.07
2108	CG1	ILE	В	608	53.550	-14.230	97.980	1.00	49.31
2109	CD1	ILE	В	608	52.448	-13.233	97.562	1.00	50.75
2110	CG2	ILE	В	608	53.146	-16.282	96.537	1.00	42.03
2111	C	ILE	В	608	55.742	-16.879	96.433	1.00	48.49
2112	0	ILE	В	608	56.251	-16.848	95.356	1.00	47.91
2113	N	HIS	В	609	55.425	-18.022	97.025	1.00	49.63
2114	CA	HIS	В	609	55.656	-19.227	96.270	1.00	51.07
2115	CB	HIS	В	609	56.018	-20.399	97.228	1.00	52.62
2116	CG	HIS	В	609	56.581	-21.599	96.510		58,.19
2117	ND1	HIS	В	609	55.816	-22.693	96.162		61.53
2118	CE1	HIS	В	609	56.579	-23.592	95.553	1.00	
2119	NE2	HIS	В	609	57.808	-23.110	95.462		68.36
2120	CD2	HIS	В	609	57.837		96.060		67.33
2121	C	HIS	В	609	54.553	-19.610	95.259		49.78
2122	0		В	609	53.384	-19.793	95.618		51.06
.2123	N		В	610		-19.951	94.060		49.31
2124	CA		В	610	54.043	-20.289	92.937		48.79
2125	CB			610		-20.868	91.902		47.24
2126	CG	PRO		610	56.241	-20.130	92.245		45.60
2127	CD	PRO		610	56.362	-20.127	93.691		48.27
2128	C	PRO		610	52.968	-21.233	93.256		47.95
2129	0	PRO		610	51.831	-21.007	92.869		49.54
2130	N	SER		611	53.307	-22.313	93.907		48.59 48.44
2131	CA	SER		611		-23.175 -24.417	94.438 95.162		51.57
2132	CB			611 611		-24.417	96.289		52.63
2133 2134	OG C			611		-24.112	95.404		47.60
2134	0	SER		611	50.501	-22.400	95.803		48.97
2136	N	CYS		612	51.820	-21.290	95.872		46.75
2137	CA			612		-20.743	96.749		48.06
2138	CB	CYS				-19.740	97.818		47.86
2139	SG			612		-20.799	98.813		51.39
2140	C .			612		-20.195	96.060		45.77
2141	Ō			612		-19.972	96.685		45.07
2142	N	VAL				-20.011	94.767		44.88
2143	CA	VAL				-19.212	94.037		44.04
2144	CB	VAL				-18.166	93.300		45.69
2145		VAL				-17.575	92.151	1.00	41.35
2146	CG2					-17.191	94.320	1.00	41.89
2147	C			613		-19.928	93.015		42.53
2148	0	VAL				-20.712	92.308		43.54
2149	N			614		-19.543	92.870	1.00	40.71
2150	CA			614		-20.229	91.985	1.00	41.54
2151	СВ			614	45.183	-21.096	92.969	1.00	40.51
2152	OG1	THR	В	614	45.217	-22.498	92.671	1.00	48.61

FIGURE 3AR

A	В	С	D	E	F	G	Н	I	J
2153	CG2	THR	В	614	43.817	-20.769	93.108	1.00	44.50
2154	С	THR	В	614	45.095	-19.149	91.179	1.00	41.38
2155	0	THR	В	614	44.528	-18.144	91.814	1.00	42.18
2156	N	ARG	В	615	44.943	-19.369	89.853	1.00	38.93
2157	CA			615		-18.494	88.956	1.00	36.43
2158	CB			615		-18.179	87.724	1.00	36.87
2159	CG			615	46.293	-17.663	87.956	1.00	35.71
2160	CD			615	47.125	-17.512	86.727	1.00	38.53
2161	NE			615		-18.840	86.152	1.00	38.81
2162	CZ			615	47.844	-19.126	84.944	1.00	38.46
2163		ARG			47.984	-20.387	84.635	1.00	31.60
2164		ARG			48.288	-18.181	84.111	1.00	33.51
2165	C			615	42.893	-19.117	88.530	1.00	37.76
2166	0 ,					-20.263	88.159	1.00	39.62
2167	N			616		-18.383	88.576	1.00	38.21
2168	CA			616		-18.954	88.262	1.00	37.39
2169	CB			616		-18.618	89.472	1:00	39.47
2170	CG			616		-19.563	90.688		43.49
2171	CD			616	39.636	-18.814	92.022	1.00	50.53
2172		GLN				-17.701	92.256	1.00	48.97
2173	NE2	GLN	В	616	38.866	-19.425	92.903	1.00	57.89
2174	С			616		-18.178	87.047	1.00	36.84
2175	0			616	38.992	-18.598	86.463	1.00	32.04
2176	N	LYS	В	617		-16.990	86.746	1.00	35.94
2177	CA	LYS	В	617		-16.287	85.725	1.00	38.36
2178	CB	LYS	В	617	38.377	-16.007	86.263	1.00	39.22
2179	CG	LYS	В	617		-14.698	86.233	1.00	42.77
2180	CD	LYS	В	617	36.370	-14.825	86.696	1.00	53.79
2181	CE	LYS	В	617	35.593	-13.466	87.025	1.00	63.68
2182	NZ	LYS	В	617	35.717	-12.927	88.489	1.00	63.21
2183	C	LYS	В	617	40.552	-15.100	85.316	1.00	40.50
2184	0	LYS	В	617	41.225	-14.556	86.140	1.00	42.28
2185	N	VAL	В	618	40.594	-14.712	84.039	1.00	40.89
2186	CA	VAL	В	618	41.186	-13.431	83.793	1.00	40.18
2187	CB	VAL	В	618 -	41.706	-13.349	82.385	1.00	40.55
2188	CG1	VAL	В	618	42.262	-11.973	82.120	1.00	44.64
2189	CG2	VAL	В	618	42.780	-14.535	82.162	1.00	41.80
2190	C	VAL	В	618	40.213	-12.346	83.975	1.00	38.00
2191	0	VAL	В	618		-12.485			39.02
2192	N	ILE	В	619	40.614	-11.229	84.559	1.00	38.05
2193	CA	ILE	В	619	39.694	-10.134		1.00	39.66
2194	CB	ILE	В	619		-9.832	86.309	1.00	40.93
2195	CG1	ILE	В	619	40.991	-9.612	86.979		38.06
2196	CD1	ILE	В	619	40.786	-9.252	88.632		36.23
2197	CG2			619		-11.004	87.102		40.94
2198	C			619	40.206	-8.870	84.202		43.93
2199	0			619	39.560	-7.812	84.237		42.87
2200	N			620	41.393		83.623		45.17
2201	CA	GLY	В	620	41.915				47.33
2202	C			620	43.224				50.85
2203	0			620	43.871		82.620		51.47
2204	N	ALA	В	621	43.595	-7.160	81.572	1.00	51.35

FIGURE 3AS

A	В	С	D	E	F	G	Н	I	J
2205	CI T	7 T 7	Б	601	44 760	7 104	00 745	1 00	53.88
2205	CA			621	44.760 44.426		80.745		54.10
2206 2207	CB			621		-7.688	79.316	1.00	
	C			621	45.299	-5.791	80.674 79.886	1.00	
2208	0			621	44.828	-4.959 -5.589			
2209	N			622	46.264 47.168		81.554		57.03 59.11
2210	CA			622		-4.483	81.562		58.66
2211	C			622 622	48.209	-4.562	80.477		59.00
2212	0				48.272	-5.501	79.641		
2213	N			623 623	49.057 50.174	-3.532	80.510 79.539		59.69 60.06
2214	CA			623		-3.401 -1.953			61.65
2215	CB				50.715		79.435 80.577		66.11
2216	CG			623	51.576	-1.387			77.25
2217	CD			623	52.456	-0.197	80.080		
2218		GLU			52.149	0.983	80.464		79.02
2219	OE2			623	53.437	-0.432	79.272		79.70
2220	C			623	51.309	-4.335	79.842	1.00	
2221	0			623	. 52.235	-4.436	79.070		60.16
2222	N			624	51.275	-5.016	80.970		54.74
2223	CA			624	52.410	-5.847	81.262		51.99
2224	CB			624	52.789	-5.730	82.754		51.88
2225	CG			624	53.391	-4.399	83.133		54.02
2226	CD1			624	54.733	-4.102	82.907		55.50
2227	CE1			624	55.256	-2.813	83.249		56.20
2228	CZ			624	54.422	-1.780	83.816		56.45
2229	CE2			624	53.062	-2.046	84.037		52.77
2230		PHE			52.556	-3.379	83.686		56.55
2231	C			624	51.975	-7.269	80.865		50.15
2232	0			624	52.725	-8.128	80.468		50.83
2233	N			625	50.672	-7.410	80.863		47.48
2234	CA	GLY			50.054	-8.656	80.601		45.33
2235	C			625	48.716	-8.751	81.302		43.78
2236	O N			625	48.093	-7.765	81.722		43.69
2237	N			626		-10.005	81.484		44.33
2238	CA	GLU				-10.291	82.001		43.81
2239	CB	GLU				-11.745	81.695		44.48
2240	CG CD	GLU GLU				-12.117	80.292		51.57 61.26
2241 2242	OE1			626		-12.312 -11.265	79.404 78.940		69.20
						-13.467	79.241		64.36
2243		GLU							40.95
2244	C	GLU				-10.078			41.04
2245	O N	GLU			45.674	-10.120	84.202		
2246	N	VAL					83.869		37.16
2247	CA	VAL VAL			45.186 44.730		85.213		35.92 34.09
2248	CB						85.610		
2249		VAL			44.433		87.155 85.273		27.95
2250		VAL				-7.191 -10.796	85.273		36.93
2251	C	VAL					85.471		35.59 37.84
2252	O N	VAL				-10.850	84.773		37.84
2253	N	TYR				-11.644			31.13
2254	CA	TYR				-12.753			31.63
2255	CB	TYR				-14.055			30.96
2256	CG	TYR	B	628	45.∠50	-14.532	85.752	T.00	30.76

FIGURE 3AT

A	В	C	D	E	F	G	Н	I	J
2257	CD1	TYR	В	628	46.561	-14.097	85.486	1.00	28.48
2258	CE1				47.279	-14.488	84.434	1.00	30.85
2259	CZ	TYR	В	628	46.688	-15.369	83.475	1.00	38.38
2260	ОН	TYR	В	628	47.394	-15.748	82.353	1.00	43.82
2261	CE2	TYR	В	628	45.377	-15.760	83.588	1.00	33.96
2262	CD2	TYR	В	628	44.636	-15.354	84.802	1.00	34.73
2263	С	TYR	В	628	43.038	-12.555	88.305	1.00	33.38
2264	0			628		-11.894	89.182	1.00	33.26
2265	N	LYS	В	629	41.975	-13.240	88.574	1.00	33.61
2266	CA	LYS	В	629	41.460	-13.260	89.864	1.00	36.43
2267	CB	LYS	В	629	39.965	-13.117	89.816	1.00	34.99
2268	CG	LYS	В	629	39.239	-14.031	90.690	1.00	42.88
2269	CD	LYS	В	629	39.362	-13.567	92.036	1.00	47.09
2270	CE	LYS	В	629	39.418	-14.774	92.959	1.00	51.42
2271	NZ	LYS	В	629	38.203	-15.510	93.282	1.00	38.62
2272	C	LYS	В	629	41.838	-14.646	90.264	1.00	38.05
2273	0	LYS	В	629	41.706	-15.573	89.484	1.00	34.96
2274	N	GLY	В	630	42.248	-14.773	91.520	1.00	39.79
2275	CA	GLY	В	630	42.714	-16.017	92.012	1.00	40.62
2276	C	GLY	В	630	42.659	-16.168	93.499	1.00	41.62
2277	0	GLY	В	630	41.952	-15.455	94.134	1.00	42.67
2278	N	MET	₿	631	43.414	-17.122	94.046	1.00	42.11
2279	CA	MET	В	631	43.374	-17.424	95.471	1.00	40.08
2280	CB	MET	В	631	42.675	-18.782	95.697	1.00	39.40
2281	CG	MET	В	631	41.244	-18.772	95.422	1.00	36.74
2282	SD	MET	В	631	40.271	-17.481	96.157	1.00	46.24
2283	CE	MET	В	631	40.094	-18.103	98.007	1.00	44.76
2284	C	MET	В	631	44.847	-17.573	95.862		40.76
2285	0	MET	В	631		-18.078	95.080		38.68
2286	N			632		-17.167	97.064		41.51
2287	CA			632		-17.311	97.497		43.33
2288	CB			632		-15.967	97.744		43.33
2289	CG			632		-15.982	98.533		39.74
2290		LEU				-16.156	97.728		38.69
2291		LEU				-14.657	99.169		41.35
2292	C			632		-18.052	98.813		47.21
2293	0			632		-17.737	99.630		46.45
2294	N	ALA				-19.043			51.87
2295	CA	ALA					100.227		56.44
2296	CB			633			100.004		56.80
2297	C			633		-19.045			57.40
2298	0			633		-18.761			56.04
2299	N			634		-18.599			61.86
2300	CA			634		-17.932			65.92
2301	CB			634		-16.513			67.32
2302	OG1			634		-16.420			67.54
2303	CG2			634		-15.309			69.80 67.85
2304	C			634		-18.840			
2305	O N			634		-19.118			70.48
2306	N			639		-20.684			68.69
2307	CA			639			105.027		66.79
2308	CB	ГХS	B	639	42.454	-19.415	105.55/	1.00	67.15

FIGURE 3AU

A	В	С	D	E	F	G	Н	I	J
2309	CG	LYS	В	639	42.933	-18.018	106.081	1.00	68.24
2310	CD			639		-17.136		1.00	74.03
2311	CE			639			108.280	1.00	
2312	NZ			639	41.868	-18.541	108.918	1.00	
2313	С			639	44.048	-20.001	103.622	1.00	65.00
2314	Ō			639		-20.547		1.00	65.73
2315	N			640	43.302	-19.082	103.006		60.87
2316	CA			640		-18.779	101.612	1.00	57.13
2317	CB			640	42.992	-19.919	100.768	1.00	58.15
2318	CG			640		-19.957		1.00	60.04
2319	CD			640	41.096	-20.995	99.392	1.00	64.28
2320	OE1			640		-21.294	99.310	1.00	63.14
2321	OE2			640		-21.522	98.604	1.00	61.98
2322	C			640	42.667	-17.575	101.332	1.00	54.89
2323	0	GLU	В	640		-17.402		1.00	53.30
2324	N			641	43.261	-16.690	100.573	1.00	49.18
2325	CA	VAL	В	641	42.508	-15.531	100.324	1.00	48.68
2326	CB	VAL	В	641	42.994	-14.411	101.085	1.00	49.50
2327	CG1	VAL	В	641	44.390	-14.089	100.811	1.00	48.06
2328	CG2	VAL	В	641	42.291	-13.327	100.489	1.00	57.76
2329	C	VAL	В	641	42.394	-15.118	98.866	1.00	45.71
2330	0	VAL	В	641	43.174	-15.525	97.986	1.00	46.28
2331	N	PRO	В	642	41.310	-14.483	98.553	1.00	43.57
2332	CA	PRO	В	642	41.105	-14.052	97.166	1.00	40.99
2333	CB	PRO	В	642	39.607	-13.620	97.182	1.00	40.42
2334	CG	PRO	В	642	39.389	-13.154	98.678		41.18
2335	CD	PRO	В	642	40.063	-14.358	99.351		42.33
2336	С	PRO	В	642	42.062	-12.898	96.773		38.73
2337	0	PRO	В	642		-12.022	97.550		38.87
2338	N			643		-12.896	95.580		36.26
2339	CA			643		-11.916	95.253		35.27
2340	CB			643		-12.558	95.411		35.78
2341	CG1			643		-12.734	96.921		33.58
2342	CG2			643		-13.818	94.815		34.92
2343	C			643		-11.546	93.775		36.64
2344	0			643		-12.389	92.922		38.44
2345	N			644		-10.326	93.428		33.63
2346				644		-10.046			33.25
2347	CB			644		-8.580	91.626		29.05
2348	C			644		-10.378	91.637		33.38
2349	0			644		-10.129			34.78
2350	N			645		-10.898			34.84
2351	CA			645		-11.220	89.994		34.70
2352	CB			645		-12.634	89.772		36.71
2353	CG1			645		-13.340	91.011 90.739		36.62 35.69
2354	CD1			645		-14.627 -13.009	89.414		36.76
2355	CG2 C			645 645		-13.009	88.716		35.66
2356 2357	0			645		-11.078	87.655		33.28
2357	N			646	48.576	-9.822	88.775		37.62
2359	CA			646		-9.156			39.51
2360	CB			646	49.392	-7.713	87.934		40.50
			_						

FIGURE 3AV

A	В	С	D	E	F	G	Ħ	I	J
2361	CG	LYS	В	646	48.112	-6.902	88.103	1.00	43.92
2362	CD	LYS	В	646	48.459	-5.427	88.516	1.00	51.47
2363	CE			646	48.982	-4.629	87.354	1.00	57.30
2364	NZ			646	49.752	-3.453	87.904		62.15
2365	C			646	50.303	-9.865	87.182	1.00	42.10
2366	0			646		-10.125	87.959		43.88
2367	N			647		-10.323	85.945		45.48
2368	CA			647		-10.990	85.290		46.92
2369	CB			647		-12.184	84.508		45.72
2370	OG1			647		-11.807	83.714		49.53
2371	CG2			647		-13.128	85.536		44.75
2372	C			647		-10.155	84.313		47.24
2372	0			647		-9.142	83.797		48.92
2374	N			648		-10.596	84.070		48.96
2375	CA			648	54.249	-9.855	83.227		50.53
2376	CB			648	55.590	-9.732	83.968		49.36
2377	CG			648	56.542	-8.585	83.642		48.99
2378	CD1			648	58.040		83.579		48.58
2379	CD1	LEU		648	56.116	-7.850	82.381		43.45
2379	CD2			648		-10.784	82.043		51.82
2381	0	LEU		648		-11.893	82.196		52.19
2382	N			649		-10.417	80.869	1.00	
2382	CA			649		-11.362	79.756	1.00	
2384	CB			649		-10.894	78.487	1.00	
2385	C			649		-11.687	79.395	1.00	
2386	0			649		-10.974	79.740	1.00	
2387	N			650		-12.811	78.718	1.00	
2388	CA			650		-13.049	78.140	1.00	
2389	CB	ALA		650		-14.433	77.525		57.04
2399	C			650		-11.965	77.057	1.00	
2390	0			650		-11.510	76.413	1.00	
2391	N			651		-11.595	76.834	1.00	
2393	CA			651		-10.553	75.873	1.00	
2394	C			651	59.312	-9.445	76.746	1.00	
2395	0			651	59.712	-8.311	76.347	1.00	
2396	N			652	59.366	-9.788	78.022		58.43
2397	CA			652	59.573	-8.682	78.940		57.59
2398	CB	TYR					80.478		54.77
2399	CG			652		-10.134			56.20
2400	CD1			652		-11.415	81.380		57.11
2400	CE1			652		-12.382	82.148		54.44
2402	CZ			652		-12.044			59.06
2402	OH			652		-13.076			65.51
2404	CE2			652		-10.787			57.44
2404	CD2			652	61.426	-9.857	81.867		54.60
2405	CDZ			652	60.713	-7.765	78.455		57.13
2406	0			652	61.890	-8.195	78.433		56.27
2407	N			653	60.253	-6.536	78.165		59.21
2408	CA			653	61.056	-5.309			61.19
2419	CB			653	60.410	-3.309 -4.127	78.740	1.00	
2410	OG1			653	58.961				63.91
2411	CG2			653	61.197		78.552		59.49
2 1 1 2	CG2	TUK	2	000	01.197	- 4.134	,0.552	1.00	JJ . 4J

FIGURE 3AW

2413 C THR B 653 62.510 -5.458 78.383 1.00 62.37 2414 O THR B 653 63.408 -5.096 77.655 1.00 63.93 2415 N ALA B 654 62.748 -6.047 79.537 1.00 65.18 2416 CA ALA B 654 64.118 -6.329 78.995 1.00 66.92 2417 CB ALA B 654 65.482 -5.184 80.915 1.00 68.35 2418 C ALA B 654 65.452 -5.259 81.675 1.00 67.15 2420 N LYS B 655 63.683 -4.123 80.723 1.00 65.70 2421 CA LYS B 655 63.683 -1.23 80.723 1.00 65.70 2422 CB LYS B 655 63.683 -1.213 80.723 1.00 65.70 2422 CB LYS B 655 62.873 -0.760 81.033 1.00 65.72 2423 CG LYS B 655 62.873 -0.760 81.419 1.00 71.	A	В	C	D	E	F	G	Н	I	J
2414 O THR B 653 63.408 -5.096 77.655 1.00 63.93 2415 N ALA B 654 62.748 -6.047 79.537 1.00 65.18 2416 CA ALA B 654 64.118 -6.339 80.065 1.00 68.35 2418 C ALA B 654 65.181 -6.632 78.995 1.00 68.35 2418 C ALA B 654 65.452 -5.259 81.675 1.00 67.15 2420 N LYS B 655 63.683 -4.123 80.723 1.00 64.02 2421 CA LYS B 655 63.683 -1.23 80.723 1.00 64.02 2422 CB LYS B 655 62.873 -0.760 81.003 1.00 64.02 2423 CG LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 62.975 0.659 81.749 1.00 61.49<	2413	С	THR	В	653	62.510	-5.458	78.383	1.00	62.37
2415 N ALA B 654 62.748 -6.047 79.537 1.00 65.18 2416 CA ALA B 654 64.118 -6.339 80.065 1.00 66.92 2417 CB ALA B 654 65.181 -6.632 78.995 1.00 68.35 2418 C ALA B 654 65.452 -5.259 81.675 1.00 68.11 2420 N LYS B 655 63.683 -1.25 81.715 1.00 64.02 2422 CB LYS B 655 63.542 -3.126 81.715 1.00 64.04 2422 CB LYS B 655 62.873 -0.760 81.031 1.00 66.52 2424 CD LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 61.719 1.600 81.419 1.00 71.15 2427 C										
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2419 O ALA B 654 65.452 -5.259 81.675 1.00 68.11 2420 N LYS B 655 63.683 -4.123 80.723 1.00 65.70 2421 CA LYS B 655 63.542 -3.126 81.715 1.00 64.02 2423 CB LYS B 655 62.873 -0.760 81.003 1.00 62.73 2424 CD LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 61.719 1.600 81.419 1.00 70.62 2425 CE LYS B 655 61.719 1.600 81.419 1.00 64.99 2426 NZ LYS B 655 61.719 1.600 81.419 1.00 64.99 2428 O LYS B 655 61.594 -2.189 82.077 1.00 64.99 2428 O LYS B 656 61.594 -2.189 82.707 1.00 65.05 2423 O ALA B 656 59.741 -3.683 81.659 1.00 65.52<										
2420 N LYS B 655 63.683 -4.123 80.723 1.00 65.70 2421 CA LYS B 655 63.542 -3.126 81.715 1.00 64.02 2422 CB LYS B 655 64.033 -1.755 81.207 1.00 64.02 2423 CG LYS B 655 62.873 -0.760 81.003 1.00 62.73 2424 CD LYS B 655 61.719 1.600 81.419 1.00 70.62 2426 NZ LYS B 655 61.431 3.073 82.018 1.00 71.15 2427 C LYS B 655 61.594 -2.189 82.707 1.00 65.05 2428 O LYS B 656 61.184 -3.849 81.273 1.00 65.65 2430 CA ALA B 656 59.741 -3.683 81.659 1.00 63.27 2431 CB ALA B 656 59.746 -4.378 83.002 1.00 63.77										
2421 CA LYS B 655 63.542 -3.126 81.715 1.00 64.04 2422 CB LYS B 655 64.033 -1.755 81.277 1.00 64.04 2423 CD LYS B 655 62.975 0.659 81.731 1.00 66.52 2426 NZ LYS B 655 61.719 1.600 81.419 1.00 70.62 2426 NZ LYS B 655 62.035 -3.062 81.945 1.00 64.99 2428 O LYS B 655 62.035 -3.062 81.945 1.00 65.02 2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.62 2430 CA ALA B 656 59.741 -3.683 81.659 1.00 63.79 2431 CB ALA B 656 59.741										
2422 CB LYS B 655 64.033 -1.755 81.277 1.00 64.04 2423 CG LYS B 655 62.873 -0.760 81.003 1.00 62.73 2424 CD LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 61.719 1.600 81.419 1.00 70.62 2426 NZ LYS B 655 62.035 -3.062 81.945 1.00 64.99 2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.05 2429 N ALA B 656 59.741 -3.849 81.273 1.00 65.05 2430 CA ALA B 656 59.741 -3.889 80.698 1.00 63.21 2431 CB ALA B 656 59.776 -4.378 83.002 1.00 63.77 2432 C									1.00	64.02
2423 CG LYS B 655 62.873 -0.760 81.003 1.00 62.73 2424 CD LYS B 655 62.975 0.659 81.731 1.00 66.52 2425 CE LYS B 655 61.719 1.600 81.419 1.00 70.62 2426 NZ LYS B 655 61.431 3.073 82.018 1.00 71.15 2427 C LYS B 655 62.035 -3.062 81.945 1.00 64.99 2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.05 2429 N ALA B 656 59.7741 -3.683 81.659 1.00 65.62 2430 CA ALA B 656 59.7741 -3.683 81.699 1.00 63.21 2431 CB ALA B 656 59.776 -4.378 83.002 1.00 63.21 2432 C ALA B 657 60.688 -5.343 83.081 1.00 62.87 2433 O ALA B 657 60.688 -5.343 83.081 1.00 62.										
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2425 CE LYS B 655 61.719 1.600 81.419 1.00 70.62 2426 NZ LYS B 655 61.431 3.073 82.018 1.00 71.15 2427 C LYS B 655 62.035 -3.062 81.945 1.00 64.99 2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.05 2430 CA ALA B 656 61.184 -3.849 81.273 1.00 63.59 2431 CB ALA B 656 59.741 -3.683 81.659 1.00 63.59 2432 C ALA B 656 59.741 -3.683 81.659 1.00 63.21 2432 C ALA B 656 59.776 -4.378 83.002 1.00 63.77 2433 O ALA B 656 59.776 -4.378 83.002 1.00 63.77 2433 O ALA B 657 60.688 -5.343 83.081 1.00 65.32 2434 N ALA B 657 60.896 -5.994 84.326 1.00 62.81<									1.00	66.52
2426 NZ LYS B 655 61.431 3.073 82.018 1.00 71.15 2427 C LYS B 655 62.035 -3.062 81.945 1.00 64.99 2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.05 2429 N ALA B 656 59.741 -3.683 81.659 1.00 63.59 2431 CB ALA B 656 59.741 -3.683 81.659 1.00 63.21 2432 C ALA B 656 59.776 -4.378 83.002 1.00 63.77 2433 O ALA B 656 59.045 -4.059 83.953 1.00 65.32 2434 N ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.891									1.00	70.62
2427 C LYS B 655 62.035 -3.062 81.945 1.00 64.99 2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.05 2429 N ALA B 656 61.184 -3.849 81.273 1.00 65.62 2430 CA ALA B 656 59.741 -3.683 81.659 1.00 63.59 2431 CB ALA B 656 59.776 -4.389 80.698 1.00 63.77 2432 C ALA B 656 59.776 -4.378 83.002 1.00 63.27 2433 O ALA B 656 59.045 -4.059 83.953 1.00 65.32 2434 N ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 60.896 -5.994 84.326 1.00 60.81 2437 C ALA B 657 60.315 -5.374 86.615 1.00 60.7		NZ	LYS	В	655	61.431	3.073		1.00	71.15
2428 O LYS B 655 61.594 -2.189 82.707 1.00 65.05 2429 N ALA B 656 61.184 -3.849 81.273 1.00 65.62 2430 CA ALA B 656 59.741 -3.683 81.659 1.00 63.59 2431 CB ALA B 656 59.776 -4.378 83.002 1.00 63.77 2432 C ALA B 656 59.776 -4.378 83.002 1.00 63.77 2433 O ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 60.896 -5.994 84.326 1.00 62.87 2437 C ALA B 657 60.921 -5.063 85.578 1.00 61.39 2437 D ALA B 657 60.921 -5.063 85.578 1.00 60.38		С				62.035	-3.062	81.945	1.00	64.99
2430 CA ALA B 656 59.741 -3.683 81.659 1.00 63.59 2431 CB ALA B 656 58.729 -4.389 80.698 1.00 63.21 2432 C ALA B 656 59.776 -4.378 83.002 1.00 63.77 2433 O ALA B 657 60.688 -5.343 83.953 1.00 62.81 2434 N ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 60.921 -5.063 85.578 1.00 62.87 2437 C ALA B 657 60.315 -5.374 86.615 1.00 60.78 2438 O ALA B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 62.852 -2.176 86.804 1.00 60.46						61.594	-2.189	82.707	1.00	65.05
2431 CB Ala B 656 58.729 -4.389 80.698 1.00 63.21 2432 C Ala B 656 59.776 -4.378 83.002 1.00 63.77 2433 O Ala B 656 59.045 -4.059 83.953 1.00 65.32 2434 N Ala B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA Ala B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB Ala B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB Ala B 657 60.921 -5.063 85.578 1.00 62.87 2437 C Ala B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 62.2560 -1.118 86.857 1.00 60.46 <td>2429</td> <td>N</td> <td>ALA</td> <td>В</td> <td>656</td> <td>61.184</td> <td>-3.849</td> <td>81.273</td> <td>1.00</td> <td>65.62</td>	2429	N	ALA	В	656	61.184	-3.849	81.273	1.00	65.62
2432 C ALA B 656 59.776 -4.378 83.002 1.00 63.77 2433 O ALA B 656 59.045 -4.059 83.953 1.00 65.32 2434 N ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 60.921 -5.063 85.578 1.00 61.39 2437 C ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.78 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.99 2440 CA VAL B 658 62.852 -2.176 86.857 1.00 60.99 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 6	2430	CA	ALA	В	656	59.741	-3.683	81.659	1.00	63.59
2433 O ALA B 656 59.045 -4.059 83.953 1.00 65.32 2434 N ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 62.153 -6.830 84.259 1.00 62.87 2437 C ALA B 657 60.921 -5.063 85.578 1.00 60.78 2438 O ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CG1 VAL B 658 62.560 -1.118 85.803 1.00 62.51 2443 CG2 VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658	2431	CB	ALA	В	656	58.729	-4.389	80.698	1.00	63.21
2434 N ALA B 657 60.688 -5.343 83.081 1.00 62.81 2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 62.153 -6.830 84.259 1.00 62.87 2437 C ALA B 657 60.921 -5.063 85.578 1.00 60.78 2438 O ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CG1 VAL B 658 62.852 -2.176 86.857 1.00 60.81 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00	2432	C	ALA	В	656	59.776	-4.378	83.002	1.00	63.77
2435 CA ALA B 657 60.896 -5.994 84.326 1.00 61.44 2436 CB ALA B 657 62.153 -6.830 84.259 1.00 62.87 2437 C ALA B 657 60.921 -5.063 85.578 1.00 60.39 2438 O ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CG1 VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 60.583 -2.403 87.005 1.00 59.81 2444 C VAL B 658 60.583 -2.403 87.005 1.00 58.61 2445 O VAL B 658 60.583 -2.289 88.146 1.00	2433	0	ALA	В	656	59.045	-4.059	83.953	1.00	65.32
2436 CB ALA B 657 62.153 -6.830 84.259 1.00 62.87 2437 C ALA B 657 60.921 -5.063 85.578 1.00 61.39 2438 O ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CG1 VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 58.911 -0.960 85.994 1.00 5	2434	N	ALA	В	657	60.688	-5.343	83.081	1.00	62.81
2437 C ALA B 657 60.921 -5.063 85.578 1.00 61.39 2438 O ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CG1 VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 59.082 1.150 84.657 1.00 62	2435	CA	ALA	В	657	60.896	-5.994	84.326	1.00	61.44
2438 O ALA B 657 60.315 -5.374 86.615 1.00 60.78 2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CGI VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 59.81 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.611 -0.274 84.666 1.00 57.85 2448 CB ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 55.40	2436	CB	ALA	В	657	62.153	-6.830	84.259	1.00	62.87
2439 N VAL B 658 61.571 -3.906 85.517 1.00 60.99 2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CG1 VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.61 2447 CA ASP B 659 58.611 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 57.696 -1.717 86.556 1.00	2437	C	ALA	В	657	60.921	-5.063	85.578	1.00	61.39
2440 CA VAL B 658 61.752 -3.219 86.804 1.00 60.46 2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CGI VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 <td>2438</td> <td>0</td> <td>ALA</td> <td>В</td> <td>657</td> <td>60.315</td> <td>-5.374</td> <td></td> <td>1.00</td> <td>60.78</td>	2438	0	ALA	В	657	60.315	-5.374		1.00	60.78
2441 CB VAL B 658 62.852 -2.176 86.857 1.00 60.81 2442 CGI VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.	2439	N	VAL	В	658	61.571	-3.906	85.517	1.00	60.99
2442 CG1 VAL B 658 64.200 -2.834 86.665 1.00 62.51 2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP <td>2440</td> <td>CA</td> <td>VAL</td> <td>В</td> <td>658</td> <td>61.752</td> <td>-3.219</td> <td>86.804</td> <td>1.00</td> <td>60.46</td>	2440	CA	VAL	В	658	61.752	-3.219	86.804	1.00	60.46
2443 CG2 VAL B 658 62.560 -1.118 85.803 1.00 62.91 2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696	2441	CB	VAL	В	658	62.852	-2.176			
2444 C VAL B 658 60.583 -2.403 87.005 1.00 59.81 2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 54.47 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30	2442									
2445 O VAL B 658 60.146 -2.289 88.146 1.00 58.61 2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.										
2446 N ASP B 659 60.080 -1.838 85.890 1.00 58.44 2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2447 CA ASP B 659 58.911 -0.960 85.994 1.00 57.85 2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2448 CB ASP B 659 58.611 -0.274 84.666 1.00 58.73 2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2449 CG ASP B 659 59.082 1.150 84.657 1.00 62.54 2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2450 OD1 ASP B 659 59.986 1.499 83.839 1.00 65.80 2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2451 OD2 ASP B 659 58.612 1.992 85.486 1.00 70.42 2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2452 C ASP B 659 57.696 -1.717 86.556 1.00 55.40 2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2453 O ASP B 659 56.889 -1.170 87.285 1.00 54.47 2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2454 N PHE B 660 57.645 -2.993 86.222 1.00 53.30 2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2455 CA PHE B 660 56.616 -3.893 86.688 1.00 51.47 2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2456 CB PHE B 660 56.687 -5.210 85.888 1.00 50.03										
2457 CG PHE B 660 55.099 -0.247 66.324 1.00 45.76										
2458 CD1 PHE B 660 54.375 -6.154 85.964 1.00 42.78										
2459 CE1 PHE B 660 53.495 -7.117 86.364 1.00 29.42										
2460 CZ PHE B 660 53.493 -7.117 86.364 1.00 25.42										
2461 CE2 PHE B 660 55.234 -8.230 87.541 1.00 34.32										
2462 CD2 PHE B 660 56.092 -7.299 87.134 1.00 41.88										
2463 C PHE B 660 56.809 -4.159 88.180 1.00 51.98										
2464 O PHE B 660 55.970 -3.826 88.979 1.00 53.32										

FIGURE 3AX

A	В	С	D	E		F	G		Н	I	J
2465	N	LEU	В	661	_	7.867	-4.818	88	.587	1.00	51.16
2466	CA	LEU				8.052	-4.986		.025	1.00	49.90
2467	CB			661		9.410	-5.608		.304	1.00	
2468	CG	LEU		661		59.401	-7.101		.967		49.47
2469	CD1	LEU		661		50.075	-7.725		.087		49.31
2470	CD2	LEU				8.040	-7.634		.013		47.87
2471	C			661		8.084	-3.654		.722		48.85
2472	Ō			661		7.712	-3.584		.846		52.10
2473	N	GLY				8.555	-2.595		.098		46.78
2474	CA	GLY				8.683	-1.340	90	.803		44.02
2475	C			662	5	57.361	-0.929		.466	1.00	45.84
2476	0			662		57.336	-0.347		.600	1.00	45.76
2477	N			663		6.258	-1.222		. 753		44.38
2478	CA			663		4.970	-0.787		.194	1.00	43.00
2479	CB	GLU		663	5	3.843	-1.079		.191	1.00	43.42
2480	CG	GLU	В	663	5	52.554	-1.313	91	.003	1.00	48.94
2481	CD	GLU	В	663	5	51.261	-1.147		.298	1.00	55.99
2482	OE1	GLU	В	663	5	50.348	-0.344	90	.786	1.00	56.46
2483	QE2	GLU	В	663	5	51.131	-1.926	89	.326	1.00	62.78
2484	С	GLU	В	663		54.735	-1.449	92	.490	1.00	40.69
2485	0	GLU	В	663	S	54.243	-0.836	93	.429	1.00	39.77
2486	N	ALA	В	664	5	55.147	-2.699	92	.549	1.00	41.23
2487	CA	ALA	В	664	5	4.964	-3.521	93	.768	1.00	42.51
2488	CB	ALA	В	664	5	55.361	-4.924	93	.525	1.00	40.07
2489	C	ALA	В	664	5	55.811	-2.917	94	.871	1.00	42.68
2490	0	ALA	В	664	5	55.438	-2.924	96	.042	1.00	43.36
2491	N	GLY	В	665	5	6.960	-2.374	94	.476	1.00	43.87
2492	CA	GLY	В	665	5	57.931	-1.819	95	.439		43.94
2493	С	GLY	В	665	5	57.330	-0.667		.169		43.52
2494	0	GLY		665		57.462	-0.519		.381		44.23
2495	N			666		66.629	0.158		.425		42.33
2496	CA	ILE		666		55.965	1.280		.055		42.70
2497	CB			666		55.513	2.167		.932		43.27
2498	CG1			666		6.724	2.800		.203		40.47
2499	CD1			666		6.305	3.460		.869		45.35
2500	CG2	ILE		666		4.692	3.137		.468		42.19
2501	C			666		4.729	0.884		.947		43.44
2502	0			666		4.624	1.234		.167		43.04
2503	N	MET				33.817	0.140		.328		42.32
2504	CA	MET				2.569	-0.368		.938		42.19
2505	CB	MET				51.932	-1.230		.817		41.53 47.32
2506	CG	MET				51.176	-2.507		.165		52.61
2507	SD	MET				19.731	-2.572		.829 .551		44.11
2508	CE	MET				0.549	-1.966 -1.095		.259		40.97
2509 2510	C	MET				52.855 52.115	-1.095		.249		40.97
2510	O	MET					-1.057		.310		41.23
2511	N CA	GLY GLY				33.973 54.340	-1.762		.534		40.60
2512 2513	CA	GLY				54.751		100			40.90
2513 2514	0	GLY				4.751	-1.869				40.12
2514 2515	N	GLN				4.995	-0.332				42.10
2515	CA			669		55.298	0.588				41.36
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FIGURE 3AY

A	В	С	D	E	F	G	H	I	J
2517	CB	GLN	В	669	55.949	1.743	100.749	1.00	40.50
2518	CG	GLN			57.369		100.440		44.93
2519	CD	GLN		669	57.848	2.816	99.700		53.63
2520	OE1	GLN			57.922		100.272		55.16
2521	NE2	GLN			58.134	2.617	98.409	1.00	51.35
2522	C			669	53.996	1.102		1.00	43.35
2523	0	GLN	В	669	54.128	1.753	103.081	1.00	45.25
2524	N	PHE	В	670	52.769	0.833	101.553	1.00	41.08
2525	CA	PHE	В	670	51.612	1.398	102.134	1.00	37.80
2526	CB	PHE	В	670	50.688	2.045	101.056	1.00	37.43
2527	CG	PHE	В	670	51.446	2.912	100.086	1.00	36.83
2528	CD1	PHE	В	670	51.220	2.868	98.724	1.00	36.12
2529	CE1	PHE	В	670	51.971	3.676	97.852	1.00	41.89
2530	CZ	PHE	В	670	52.941	4.539	98.359	1.00	43.63
2531	CE2	PHE	В	670	53078	4.636	99.746	1.00	39.81
2532	CD2	PHE	В	670	52.356	3.822		1.00	34.13
2533	C	PHE	В	670	50.888	0.359		1.00	35.75
2534	0	PHE	В	670	51.117	-0.756			31.50
2535	N	SER		671	50.178	0.774	103.923		35.37
2536	CA	SER		671	49.179		104.556		35.63
2537	CB			671	49.795		105.584		37.05
2538	OG			671	48.754	-1.432			35.05
2539	С			671	48.009	0.915			35.05
2540	0			671	48.061	1.604			36.76
2541	N			672	46.930	0.915			33.56
2542	CA	HIS			45.871		104.659		34.12
2543	CB	HIS			46.232	3.243			32.36
2544	CG	HIS			45.251	4.288			33.02
2545		HIS			44.080		103.586		33.28
2546		HIS			43.406	5.471			34.10
2547		HIS			44.044	5.886		1.00	
2548	CD2	HIS HIS			45.198 44.633	5.161 1.308			33.03
2549 2550					44.633		104.017		33.41
2550 2551	O N	HIS HIS			43.502	1.611			30.53
2552	CA	HIS		673	42.230	1.011			31.97
2552	CB	HIS			41.296	1.817			30.58
2554	CG				39.877		105.083		37.08
2555		HIS			39.369		105.415		42.49
2556		HIS			38.051		105.241		43.15
2557		HIS			37.690		104.828		31.71
2558		HIS			38.814		104.721		39.22
2559	C	HIS			41.832		102.843		33.87
2560	0	HIS			40.989		102.229		34.38
2561	N	ASN			42.323		102.363		33.75
2562	CA	ASN			41.797		101.126		32.88
2563	CB	ASN			41.166		101.219		30.97
2564	CG	ASN			39.921		102.092		31.43
2565		ASN			38.806		101.636		30.88
2566		ASN			40.022	5.112	103.273	1.00	20.74
2567	C	ASN			42.854		100.080		31.69
2568	0	ASN			42.730	3.587	99.082	1.00	30.93

FIGURE 3AZ

A	В	С	D	E	F	G	Н	I	J
2569	N	ILE	В	675	43.861	2.055	100.334	1.00	31.51
2570	CA	ILE	В	675	44.993	1.813	99.460	1.00	30.93
2571	CB	ILE	В	675	46.273	2.205	100.110	1.00	31.44
2572	CG1	ILE	В	675	46.250	3.687	100.454	1.00	28.51
2573	CD1	ILE		675	46.340	4.549	99.164		31.74
2574	CG2	ILE		675	47.486	2.026	99.005		22.20
2575	C	ILE		675	45.052	0.297	99.215		34.26
2576	0	ILE	В	675	44.924	-0.515	100.144	1.00	36.44
2577	N	ILE		676	45.186	-0.100	97.964	1.00	34.31
2578	CA	ILE	В	676	44.977	-1.451	97.663	1.00	34.35
2579	CB	ILE	В	676	44.919	-1.703	96.111	1.00	35.23
2580	CG1	ILE	В	676	44.509	-3.132	95.837	. 1.00	35.18
2581	CD1	ILE	В	676	42.941	-3.264	96.042	1.00	39.25
2582	CG2	ILE	В	676	46.229	-1.573	95.495	1.00	35.77
2583	С	ILE		676	46.143	-2.067	98.326	1.00	34.50
2584	0	ILE		676	47.226	-1.536	98.234	1.00	33.39
2585	N	ARG	В	677	45.933	-3.239	98.897	1.00	33.92
2586	CA	ARG	В	677	46.961	-3.942	99.559	1.00	33.57
2587	CB	ARG	В	677	46.317	-4.719	100.700	1.00	32.83
2588	CG	ARG	В	677	47.392	-5.572	101.445	1.00	35.49
2589	CD	ARG		677	46.901	-6.224	102.708	1.00	47.46
2590	NE	ARG	В	677	45.887	-7.206	102.394	1.00	52.58
2591	CZ	ARG	В	677	44.635	-7.100	102.814	1.00	59.96
2592	NH1	ARG	В	677	44.304	-6.024	103.587	1.00	55.86
2593	NH2	ARG	В	677	43.742	-8.063	102.463	1.00	56.27
2594	C	ARG	В	677	47.797	-4.926	98.720	1.00	34.17
2595	0	ARG	В	677	47.229	-5.704	97.993	1.00	36.51
2596	N	LEU	В	678	49.115	-4.899	98.837	1.00	33.13
2597	CA	LEU	В	678	50.033	-5.811	98.197	1.00	37.40
2598	CB	LEU	В	678	51.435	-5.236	98.159	1.00	36.36
2599	CG	LEU	В	678	52.397	-6.185	97.415	1.00	42.53
2600	CD1	LEU	В	678	51.911	-6.418	95.980	1.00	35.69
2601	CD2	LEU	В	678	53.852	-5.640	97.304	1.00	41.94
2602	C	LEU	В	678	50.171	-7.067	99.042	1.00	39.09
2603	0	LEU	В	678	50.517	-6.970	100.188	1.00	40.71
2604	N	GLU	В	679	49.836	-8.226	98.507	1.00	41.09
2605	CA	GLU	В	679	49.976	-9.417	99.253	1.00	42.38
2606	CB	GLU	В	679	49.026	-10.474	98.789	1.00	41.41
2607	CG	GLU	В	679			99.081	1.00	45.00
2608	CD	GLU	В	679	47.179	-10.261	100.578	1.00	51.76
2609	OE1	GLU	В	679		-11.040		1.00	52.41
2610	OE2	GLU	В	679	46.290	-9.498	101.008	1.00	55.14
2611	C	GLU	В	679		-9.866		1.00	42.27
2612	0	GLU	В	679	51.912	-10.278	100.108	1.00	44.77
2613	N	GLY	В	680	51.973	-9.623	97.972	1.00	41.28
2614	CA	GLY	В	680		-10.180	97.623		41.26
2615	C	GLY	В	680	53.582	-10.240	96.127	1.00	42.91
2616	0	GLY	В	680		-9.669	95.349		42.87
2617	N	VAL	В	681		-10.893	95.716		44.63
2618	CA			681		-10.858	94.316		47.33
2619	CB			681		-9.792	93.916		47.94
2620		VAL				-8.411	94.202		48.45
2621	CG2	VAL				-10.075			47.53
2622	С	VAL	В	681	55.811	-12.121	94.003	1.00	49.45

FIGURE 3BA

2623 O VAL B 681 56.375 -12.823 94.891 1.00 48.56 2624 N ILE B 682 55.785 -12.422 92.707 1.00 50.88 2625 CA ILE B 682 56.648 -13.445 92.194 1.00 52.35 2626 CB ILE B 682 56.040 -14.781 92.219 1.00 52.57 2627 CG1 ILE B 682 54.614 -14.850 91.771 1.00 54.23 2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45 2641 C ALA B 684 62.426 -16.045 92.155 1.00 65.59	A	В	С	D	E	F	G	Н	I	J
2624 N ILE B 682 55.785 -12.422 92.707 1.00 50.88 2625 CA ILE B 682 56.648 -13.445 92.194 1.00 52.35 2626 CB ILE B 682 56.040 -14.781 92.219 1.00 52.57 2627 CG1 ILE B 682 54.614 -14.850 91.771 1.00 54.23 2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 65.44	2623	0	VAL	В	681	56.375	-12.823	94.891	1.00	48.56
2625 CA ILE B 682 56.648 -13.445 92.194 1.00 52.35 2626 CB ILE B 682 56.040 -14.781 92.219 1.00 52.57 2627 CG1 ILE B 682 54.614 -14.850 91.771 1.00 54.23 2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.4										
2626 CB ILE B 682 56.040 -14.781 92.219 1.00 52.57 2627 CG1 ILE B 682 54.614 -14.850 91.771 1.00 54.23 2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 61.114 -12.079 92.783 1.00 64.03 2635 OG <										
2627 CG1 ILE B 682 54.614 -14.850 91.771 1.00 54.23 2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2639 CA ALA B 684 61.921 -14.287 90.467 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45						56.040	-14.781			
2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2637 O SER B 683 60.691 -14.088 90.824 1.00 60.75 2638 N						54.614	-14.850			
2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45							_			
2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2634 CB SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2635 OG SER B 683 61.114 -12.079 92.783 1.00 64.03 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2640 CB ALA B 684 62.426 -16.045 92.155 1.00 65.45										
2641 C ALA B 684 61.607 -16.690 89.844 1.00 65.59	2641	C						89.844		
2642 O ALA B 684 62.156 -17.667 89.411 1.00 66.62										
2643 N TYR B 685 60.320 -16.489 89.629 1.00 65.92										
2644 CA TYR B 685 59.566 -17.433 88.808 1.00 65.61										
2645 CB TYR B 685 58.513 -18.132 89.646 1.00 66.23										
2646 CG TYR B 685 59.148 -19.196 90.468 1.00 69.68										
2647 CD1 TYR B 685 59.519 -18.961 91.769 1.00 67.64										
2648 CE1 TYR B 685 60.131 -19.935 92.519 1.00 71.61										
2649 CZ TYR B 685 60.433 -21.157 91.970 1.00 74.46										
2650 OH TYR B 685 61.042 -22.113 92.750 1.00 75.04										
2651 CE2 TYR B 685 60.081 -21.448 90.663 1.00 75.00										
2652 CD2 TYR B 685 59.446 -20.453 89.905 1.00 75.26										
2653 C TYR B 685 58.964 -16.788 87.581 1.00 65.25										65.25
2654 O TYR B 685 58.899 -15.527 87.499 1.00 66.17								87.499		
2655 N ALA B 686 58.551 -17.617 86.612 1.00 63.68									1.00	63.68
2656 CA ALA B 686 58.036 -17.091 85.334 1.00 62.32		CA				58.036	-17.091			
2657 CB ALA B 686 58.506 -17.805 84.124 1.00 63.30		CB	ALA	В	686	58.506	-17.805	84.124	1.00	63.30
2658 C ALA B 686 56.596 -17.082 85.432 1.00 62.05	2658	С	ALA	₿	686			85.432	1.00	62.05
2659 O ALA B 686 56.007 -18.119 85.775 1.00 63.53		0				56.007			1.00	63.53
2660 N PRO B 687 56.081 -16.278 84.593 1.00 60.53		N	PRO	В	687	56.081	-16.278	84.593	1.00	60.53
2661 CA PRO B 687 55.343 -15.047 84.649 1.00 58.99						55.343	-15.047		1.00	58.99
2662 CB PRO B 687 53.882 -15.447 84.418 1.00 58.56	2662	CB	PRO	В	687	53.882	-15.447	84.418	1.00	58.56
2663 CG PRO B 687 53.888 -16.897 84.821 1.00 60.26		CG	PRO	В	687			84.821	1.00	60.26
2664 CD PRO B 687 55.173 -17.326 84.077 1.00 61.17	2664	CD	PRO	В	687	55.173	-17.326	84.077	1.00	61.17
2665 C PRO B 687 55.589 -14.602 86.037 1.00 56.90	2665	C	PRO	В	687	55.589	-14.602	86.037	1.00	56.90
2666 O PRO B 687 55.308 -15.358 86.974 1.00 56.82	2666	0	PRO	В	687	55.308	-15.358		1.00	56.82
2667 N MET B 688 56.186 -13.428 86.143 1.00 55.27		N	MET	В	688	56.186	-13.428		1.00	55.27
2668 CA MET B 688 56.320 -12.750 87.404 1.00 54.44		CA							1.00	54.44
2669 CB MET B 688 57.223 -11.566 87.255 1.00 55.33										
2670 CG MET B 688 58.596 -11.932 86.692 1.00 55.74										
2671 SD MET B 688 59.901 -11.043 87.530 1.00 60.68										
2672 CE MET B 688 60.394 -9.447 86.370 1.00 57.44										
2673 C MET B 688 54.924 -12.281 87.695 1.00 53.73										
2674 O MET B 688 54.115 -11.957 86.766 1.00 55.62										
2675 N MET B 689 54.593 -12.326 88.964 1.00 49.82										
2676 CA MET B 689 53.314 -11.945 89.372 1.00 45.50										

FIGURE 3BB

2677 CB MET B 689	A	В	С	D	E	F	G	Н	I	J
2678 CG	2677	СВ	MET	В	689	52.726	-13.198	89.919	1.00	46.09
2680 CE MET B 689 50.901 -15.633 89.528 1.00 50.11 2681 C MET B 689 50.901 -16.233 88.146 1.00 42.03 2682 O MET B 689 53.460 -10.868 91.193 1.00 43.66 2684 CA ILE B 690 52.2546 -9.929 90.420 1.00 40.55 2685 CB ILE B 690 52.255 -7.585 90.904 1.00 41.79 2686 CGI ILE B 690 53.591 -6.955 90.607 1.00 40.50 2687 CDI ILE B 690 53.591 -6.955 90.607 1.00 38.75 2689 C ILE B 690 50.932 -9.386 91.90 1.00 38.72 2691 M ILE B 691 49.581<										
2680 CE MET B 689 50.901 -16.233 88.146 1.00 42.03 2681 C MET B 689 53.460 -10.876 90.439 1.00 43.444 2683 N ILE B 690 52.358 -8.991 91.483 1.00 43.05 2684 CB ILE B 690 52.358 -8.991 91.483 1.00 43.05 2685 CB ILE B 690 53.596 -6.955 90.904 1.00 40.50 2688 CG2 ILE B 690 53.591 -5.528 89.890 1.00 37.73 2688 CG2 ILE B 690 53.550 -5.228 89.890 1.00 38.75 2698 C ILE B 690 49.971 -9.343 91.986 1.00 38.75 2691 D ILE B 691 49.587<										
2681 C MET B 689 53.460 -10.876 90.439 1.00 44.44 2682 O MET B 689 54.468 -10.868 91.193 1.00 43.66 2684 CA ILE B 690 52.245 -7.585 90.904 1.00 40.55 2686 CGI ILE B 690 52.225 -7.585 90.904 1.00 41.79 2686 CGI ILE B 690 53.596 -6.955 90.607 1.00 37.73 2689 C ILE B 690 53.501 -5.528 89.890 1.00 38.75 2689 C ILE B 690 50.932 -9.383 91.955 1.00 38.77 2690 C ILE B 691 49.587 -10.294 91.92 1.00 33.73 2693 CB ILE B 691 49.587 <td></td>										
2682 O MET B 690 52.546 -9.929 90.420 1.00 43.66 2684 CA ILE B 690 52.358 -8.991 91.483 1.00 39.05 2685 CB ILE B 690 52.358 -8.991 91.483 1.00 41.79 2686 CGI ILE B 690 53.596 -6.955 90.607 1.00 41.79 2687 CDI ILE B 690 53.501 -5.528 89.890 1.00 37.73 2688 CG2 ILE B 690 50.932 -9.386 91.986 1.00 38.72 2690 O ILE B 691 49.587 -10.296 93.856 1.00 37.73 2693 CB ILE B 691 49.587 -10.296 93.856 1.00 37.73 2694 CGI ILE B 691 49.5										
2683 N ILE B 690 52.546 -9.929 90.420 1.00 40.55 2684 CA ILE B 690 52.358 -8.991 91.483 1.00 39.05 2686 CB ILE B 690 52.255 -7.585 90.904 1.00 41.79 2688 CG2 ILE B 690 53.501 -5.528 89.890 1.00 37.73 2688 CG2 ILE B 690 50.932 -9.386 91.986 1.00 38.72 2690 O ILE B 691 49.971 -9.343 91.92 1.00 36.41 2691 N ILE B 691 49.587 -10.296 93.856 1.00 37.73 2693 CB ILE B 691 49.587 -10.296 93.856 1.00 37.73 2694 CG1 ILE B 691 49.587 -10.296 93.856 1.00 37.57 2695 CD ILE B 691 49.587 -10.296 93.759 1.00 43.25										
2684 CA ILE B 690 52.358 -8.991 91.483 1.00 39.05 2685 CB ILE B 690 52.225 -7.585 90.904 1.00 41.79 2687 CDI ILE B 690 53.596 -6.955 90.607 1.00 40.50 2688 CG2 ILE B 690 53.501 -5.528 89.890 1.00 37.73 2689 C ILE B 690 50.932 -9.386 91.986 1.00 38.75 2690 O ILE B 690 49.971 -9.343 91.192 1.00 38.72 2691 N ILE B 691 49.971 -9.343 91.192 1.00 38.72 2693 CB ILE B 691 49.987 -10.296 93.855 1.00 37.73 2693 CB ILE B 691 49.580 -11.537 94.642 1.00 37.57 2694 CG1 ILE B 691 49.966 -12.539 93.759 1.00 43.72 2695 CDL ILE B 691 49.662 -12.539 93.759 1.00 43.73 2696 CG2 ILE B 691 48.666 -12.175 95.178 1.00 33.75 2697 C ILE B 691 48.662 -12.539 95.803 1.00 34.36 <										
2685 CB ILE B 690 52.225 -7.585 90.904 1.00 41.79 2686 CGI ILE B 690 53.596 -6.955 90.607 1.00 40.50 2688 CG2 ILE B 690 53.501 -5.528 89.890 1.00 38.75 2689 C ILE B 690 50.932 -9.386 91.986 1.00 38.75 2690 O ILE B 691 50.807 -9.788 93.255 1.00 36.41 2691 N ILE B 691 49.587 -10.296 93.856 1.00 37.73 2693 CB ILE B 691 49.587 -10.296 93.856 1.00 37.57 2694 CG1 ILE B 691 49.587 -10.296 93.856 1.00 37.57 2695 CD1 ILE B 691 49.780 -13.030 92.551 1.00 37.78 2697 C ILE B 691 49.621 -8.935 95.803 1.00 33.95 2697 C										
2686 CG1 ILE B 690 53.596 -6.955 90.607 1.00 40.50 2687 CD1 ILE B 690 53.501 -5.528 89.890 1.00 37.73 2689 C ILE B 690 50.932 -9.386 91.986 1.00 38.72 2690 O ILE B 690 49.971 -9.343 91.192 1.00 36.41 2691 N ILE B 691 49.587 -10.296 93.856 1.00 37.73 2693 CB ILE B 691 49.587 -10.296 93.856 1.00 37.57 2693 CB ILE B 691 49.581 -13.030 92.551 1.00 43.22 2695 CDI ILE B 691 48.666 -12.175 95.178 1.00 37.58 2695 CDI ILE B 691 48.										
2687 CD1 ILE B 690 53.501 -5.528 89.890 1.00 37.73 2688 CG2 ILE B 690 50.932 -9.386 91.986 1.00 38.72 2690 O ILE B 690 49.971 -9.343 91.192 1.00 38.72 2691 N ILE B 691 50.807 -9.788 93.255 1.00 38.28 2692 CA ILE B 691 49.9587 -10.296 93.856 1.00 37.57 2693 CB ILE B 691 49.780 -13.030 92.551 1.00 43.78 2696 CG2 ILE B 691 49.621 -8.935 95.803 1.00 33.95 2697 C ILE B 691 49.621 -8.935 95.803 1.00 34.36 2698 O ILE B 691 49.621										
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2714 O GLU B 693 42.890 -7.067 95.588 1.00 35.55 2715 N TYR B 694 41.845 -8.911 96.272 1.00 32.10 2716 CA TYR B 694 40.970 -8.809 95.150 1.00 28.28 2717 CB TYR B 694 40.440 -10.153 94.874 1.00 28.39 2718 CG TYR B 694 39.351 -10.217 93.769 1.00 32.24 2719 CD1 TYR B 694 39.617 -9.921 92.416 1.00 28.95 2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538		C	GLU					96.364	1.00	35.07
2715 N TYR B 694 41.845 -8.911 96.272 1.00 32.10 2716 CA TYR B 694 40.970 -8.809 95.150 1.00 28.28 2717 CB TYR B 694 40.440 -10.153 94.874 1.00 28.39 2718 CG TYR B 694 39.351 -10.217 93.769 1.00 32.24 2719 CD1 TYR B 694 39.617 -9.921 92.416 1.00 28.95 2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 39.814 -7.896 95.538 1.00 28.69 2725 C TYR B 694 39.243 -8.023 96.662 <td></td> <td></td> <td>GLU</td> <td>В</td> <td>693</td> <td></td> <td></td> <td>95.588</td> <td>1.00</td> <td>35.55</td>			GLU	В	693			95.588	1.00	35.55
2716 CA TYR B 694 40.970 -8.809 95.150 1.00 28.28 2717 CB TYR B 694 40.440 -10.153 94.874 1.00 28.39 2718 CG TYR B 694 39.351 -10.217 93.769 1.00 32.24 2719 CD1 TYR B 694 39.617 -9.921 92.416 1.00 28.95 2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 39.814 -7.896 95.538 1.00 28.69 2725 C TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99		N					-8.911		1.00	32.10
2717 CB TYR B 694 40.440 -10.153 94.874 1.00 28.39 2718 CG TYR B 694 39.351 -10.217 93.769 1.00 32.24 2719 CD1 TYR B 694 39.617 -9.921 92.416 1.00 28.95 2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99	2716					40.970	-8.809	95.150	1.00	28.28
2718 CG TYR B 694 39.351 -10.217 93.769 1.00 32.24 2719 CD1 TYR B 694 39.617 -9.921 92.416 1.00 28.95 2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99		CB				40.440	-10.153	94.874	1.00	28.39
2719 CD1 TYR B 694 39.617 -9.921 92.416 1.00 28.95 2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99		CG						93.769	1.00	32.24
2720 CE1 TYR B 694 38.566 -10.081 91.432 1.00 33.82 2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99	2719							92.416	1.00	28.95
2721 CZ TYR B 694 37.375 -10.533 91.790 1.00 31.62 2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99		CE1	TYR	В	694	38.566	-10.081	91.432	1.00	33.82
2722 OH TYR B 694 36.297 -10.655 90.899 1.00 37.93 2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99		CZ.	TYR	В	694	37.375	-10.533	91.790	1.00	31.62
2723 CE2 TYR B 694 37.108 -10.758 93.113 1.00 35.35 2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99			TYR	В	694			90.899	1.00	37.93
2724 CD2 TYR B 694 38.076 -10.619 94.080 1.00 35.75 2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99						37.108	-10.758		1.00	35.35
2725 C TYR B 694 39.814 -7.896 95.538 1.00 28.69 2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99									1.00	35.75
2726 O TYR B 694 39.243 -8.023 96.662 1.00 28.77 2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99	2725	C				39.814	-7.896	95.538	1.00	28.69
2727 N MET B 695 39.475 -6.996 94.627 1.00 25.99		0				39.243		96.662	1.00	28.77
		N	MET	В	695	39.475	-6.996	94.627	1.00	25.99
	2728	CA	MET	В	695	38.480	-6.015	94.790	1.00	28.69

FIGURE 3BC

A	В	С	D	E	F	G	Н	I	J
2729	СВ	MET	B	695	39.057	-4.593	94.582	1.00	27.01
2723	CG	MET		695	40.089	-4.121	95.806	1.00	
2731	SD	MET		695	39.137	-4.002	97.332	1.00	
2732	CE	MET		695	38.140	-2.317	96.950	1.00	19.49
2733	C	MET		695	37.337	-6.451	93.887	1.00	30.89
2734	Ō	MET			37.371	-6.254	92.716	1.00	35.87
2735	N	GLU			36.406	-7.188	94.437	1.00	31.23
2736	CA	GLU			35.369	-7.846	93.720	1.00	32.82
2737	СВ	GLU			34.419	-8.666	94.666	1.00	30.79
2738	CG	GLU	В	696	33.717	-7.643	95.469	1.00	38.13
2739	CD	GLU	В	696	33.271	-8.107	96.846	1.00	48.34
2740	OE1	GLU	В	696	32.877	-9.291	96.897	1.00	61.33
2741	OE2	GLU	В	696	33.160	-7.330	97.803	1.00	43.84
2742	C	GLU	В	696	34.529	-7.028	92.836	1.00	32.02
2743	0	GLU	₿	696	33.781	-7.625	92.021	1.00	31.01
2744	N	ASN	В	697	34.505	-5.694	92.943	1.00	33.21
2745	CA	ASN	В	697	33.694	-4.999	91.904	1.00	31.07
2746	CB	ASN	В	697	32.725	-4.026	92.537	1.00	30.83
2747	CG	ASN	В	697	31.440	-4.657	92.940	1.00	34.34
2748	OD1	ASN	В	697	30.947	-5.594	92.243	1.00	34.99
2749	ND2	ASN	В	697	30.834	-4.156	94.055	1.00	
2750	C	ASN	В	697	34.630	-4.265	90.926	1.00	31.59
2751	0	ASN	В	697	34.193	-3.413	90.103	1.00	31.69
2752	N	GLY	В	698	35.910	-4.526	90.990	1.00	29.27
2753	CA	GLY	В	698	36.768	-3.815	90.060	1.00	29.77
2754	C	GLY		698	36.882	-2.261	90.054		29.16
2755	0	GLY			36.746	-1.550	91.056	1.00	
2756	N	ALA			37.160	-1.773	88.888	1.00	
2757	CA	ALA			37.387	-0.402	88.524	1.00	
2758	CB	ALA		699	37.888	-0.293	87.086		25.30
2759	C	ALA		699	36.179	0.215	88.629		27.91
2760	0	ALA		699	35.168	-0.299	88.130	1.00	
2761	N	LEU		700	36.280	1.357	89.268	1.00	
2762	CA	LEU		700	35.121	2.026	89.707	1.00	
2763	CB	LEU		700	. 35.450	3.069	90.838	1.00	
2764	CG	LEU		700	34.459	4.089	91.301	1.00	
2765		LEU		700	33.464	3.627	92.353		30.61
2766		LEU			35.145	5.322	91.920		28.14
2767	C	LEU			34.449	2.671	88.617		30.67
2768	0	LEU		700	33.279	2.926	88.812		32.59
2769	N	ASP		701	35.175	3.092	87.584		28.67
2770	CA	ASP		701	34.475	3.801	86.542		33.44 33.00
2771	CB	ASP		701	35.382	4.505			38.53
2772	CG	ASP		701	36.230	3.542	84.702		
2773		ASP		701	36.810	2.573	85.221 83.440		37.75 40.32
2774		ASP		701	36.395	3.751			33.01
2775 2776	C	ASP		701	33.529 32.301	2.791 3.048	85.837 85.715		32.42
	O N	ASP LYS		701 702	34.074	1.635	85.538		30.90
2777	N CA	LYS		702	33.249	0.568	84.960		35.12
2778	CB					-0.548	84.449		37.12
2779		LYS			34.186		83.686		47.55
2780	CG	LYS	Þ	/ UZ	33.542	-1.537	03.000	1.00	٠,.JJ

FIGURE 3BD

A	В	С	D	E	F	G	Н	I	J
2781	CD	LYS	В	702	34.296	-2.821	83.631	1.00	60.43
2782	CE	LYS		702	33.493	-3.758	82.740	1.00	63.91
2783	NZ	LYS		702	34.151	-5.137	82.655	1.00	69.98
2784	С	LYS		702	32.158	0.088	85.872	1.00	35.34
2785	0	LYS		702	31.006	-0.038	85.504	1.00	36.22
2786	N	PHE		703	32.421	-0.020	87.179	1.00	37.97
2787	CA	PHE		703	31.403	-0.517	88.060	1.00	34.72
2788	CB	PHE	В	703	31.980	-0.605	89.436	1.00	35.11
2789	CG	PHE	В	703	30.985	-0.877	90.473	1.00	29.25
2790	CD1	PHE	В	703	30.252	-2.115	90.505	1.00	27.25
2791	CE1	PHE	В	703	29.389	-2.361	91.525	1.00	29.92
2792	CZ	PHE	В	703	29.256	-1.467	92.569	1.00	29.83
2793	CE2	PHE	В	703	29.913	-0.313	92.538	1.00	29.77
2794	CD2	PHE		703	30.785	0.001	91.443	1.00	30.63
2795	С	PHE	В	703	30.265	0.452	88.121	1.00	36.80
2796	0	PHE	В	703	29.032	0.086	88.137	1.00	37.46
2797	N	LEU	В	704	30.622	1.724	88.157	1.00	36.09
2798	CA	LEU	В	704	29.567	2.730	88.283	1.00	35.58
2799	CB	LEU	В	704	30.162	4.112	88.554	1.00	36.04
2800	CG	LEU	В	704	30.722	4.526	89.921	1.00	39.33
2801	CD1	LEU	В	704	31.453	5.870	89.856	1.00	39.49
2802	CD2	LEU	B	704	29.689	4.488	91.097	1.00	39.49
2803	C	LEU	В	704	28.723	2.859	87.005	1.00	35.48
2804	0	LEU	В	704	27.545	3.304	87.050	1.00	36.13
2805	N	ARG	В	705	29.342	2.607	85.865	1.00	36.71
2806	CA	ARG	В	705	28.645	2.652	84.601	1.00	37.41
2807	CB	ARG	В	705	29.599	2.330	83.433	1.00	37.84
2808	CG	ARG	В	705	30.260	3.590	82.802	1.00	34.77
2809	CD	ARG	В	705	30.660	3.455	81.367	1.00	41.95
2810	NE	ARG	В	705	31.988	2.810	81.271	1.00	42.52
2811	CZ	ARG	В	705	33.068	3.374	81.792	1.00	45.05
2812	NH1	ARG	В	705	34.261	2.852	81.678	1.00	42.04
2813	NH2	ARG	В	705	32.913	4.565	82.399	1.00	40.02
2814	C	ARG	В	705	27.609	1.598	84.550		40.12
2815	0	ARG	В	705	26.733	1.639	83.716		43.46
2816	N	GLU	В	706	27.773	0.561	85.322		41.24
2817	CA	GLU		706	26.916	-0.555	85.216		43.79
2818	CB	GLU	В	706	27.684	-1.832	85.558		46.45
2819	CG	GLU	В	706	28.385	-2.583	84.416		53.31
2820	CD	GLU	В	706	29.070	-3.871	85.011		65.10
2821	OE1	GLU	В	706	28.273	-4.757	85.532		68.07
2822	OE2			706	30.368	-4.034	84.995		63.05
2823	C	GLU	В	706	25.852	-0.364	86.216		43.47
2824	0	GLU	В	706	24.864	-1.051	86.164		45.43
2825	N	LYS		707	26.029	0.565	87.117		43.14
2826	CA	LYS		707	25.013	0.851	88.098		44.44
2827	CB	LYS	В	707	25.584	0.449	89.490		46.43
2828	CG	LYS	В	707	26.172	-1.029	89.491		44.84
2829	CD	LYS	В	707	25.573	-1.880	90.569		43.24
2830	CE	LYS	В	707	25.352	-3.405	90.147		48.65
2831	NZ			707	24.010	-3.911	90.629		46.05
2832	C	LYS	В	707	24.448	2.319	88.048	1.00	43.63

FIGURE 3BE

A	В	С	D	E	F	G	Н	I	J
2833	0	LYS	В	707	23.968	2.911	89.012	1.00	43.30
2834	N	ASP	В	708	24.510	2.886	86.899	1.00	43.40
2835	CA	ASP		708	24.061	4.208	86.688	1.00	45.41
2836	CB	ASP		708	23.816	4.329	85.214	1.00	45.17
2837	CG	ASP	В	708	23.571	5.756	84.769	1.00	51.04
2838	OD1	ASP	В	708	23.369	5.861	83.513	1.00	56.65
2839	OD2	ASP	В	708	23.578	6.789	85.536	1.00	50.26
2840	С	ASP	В	708	22.776	4.514	87.400	1.00	46.40
2841	0	ASP	В	708	21.809	3.760	87.256	1.00	48.89
2842	N	GLY	В	709	22.748	5.610	88.155	1.00	45.59
2843	CA	GLY		709	21.516	6.076	88.791	1.00	45.68
2844	C	GLY	В	709	21.043	5.454	90.056	1.00	45.97
2845	0	GLY	В	709	20.134	5.987	90.790	1.00	45.98
2846	N	GLU	В	710	21.713	4.355	90.402	1.00	46.33
2847	CA	GLU	В	710	21.266	3.524	91.498	1.00	44.07
2848	CB	GLU	В	710	21.639	2.091	91.156	1.00	43.37
2849	CG	GLU	В	710	21.240	1.530	89.788	1.00	45.17
2850	CD	GLU	В	710	21.407	0.012	89.910	1.00	50.33
2851	OE1	GLU	В	710	21.591	-0.451	91.103	1.00	57.24
2852	OE2	GLU	В	710	21.522	-0.675	88.894	1.00	45.95
2853	C	GLU	В	710	21.845	3.640	92.888	1.00	45.39
2854	0	GLU	В	710	21.521	2.760	93.718	1.00	47.34
2855	N	PHE	В	711	22.760	4.543	93.196	1.00	43.13
2856	CA	PHE	В	711	23.200	4.589	94.566	1.00	40.55
2857	CB	PHE	В	711	24.679	4.658	94.597	1.00	39.03
2858	CG	PHE	В	711	25.276	3.409	94.246	1.00	42.05
2859	CD1	PHE	В	711	26.050	3.281	93.108	1.00	38.47
2860	CE1	PHE	В	711	26.599	2.064	92.802	1.00	39.65
2861	CZ	PHE		711	26.275	0.880	93.622	1.00	41.38
2862	CE2	PHE	В	711	25.452	1.062	94.740	1.00	34.06
2863	CD2	PHE	В	711	24.989	2.245	95.050	1.00	37.46
2864	C	PHE	В	711	22.626	5.863	95.009	1.00	40.79
2865	0	PHE	В	711	22.154	6.588	94.204	1.00	41.46
2866	N	SER		712	22.638	6.126	96.287	1.00	42.27
2867	CA	SER		712	22.217	7.392	96.828	1.00	43.06
2868	CB	SER		712	22.065	7.169	98.297	1.00	41.23
2869	OG	SER		712	23.405	7.227	98.787	1.00	
2870	C	SER		712	23.457	8.292	96.753		43.66
2871	0	SER		712	24.613	7.773	96.636		45.02
2872	N	VAL			23.235	9.574	96.953		42.17
2873	CA	VAL			24.207	10.574	96.853		42.95
2874	CB	VAL			23.524	11.961	97.062		44.89
2875		VAL			24.513	13.096	97.189		44.06
2876		VAL		713	22.675	12.272	95.826		48.34 43.30
2877	C	VAL		713	25.151	10.328	97.995 97.881		43.30
2878	O N	VAL		713 714	26.361	10.633 9.742	99.082		42.36
2879	N Ca	LEU		714	24.607 25.412		100.294		42.34
2880	CA CB	LEU		714	25.412 24.549	9.441	100.294		41.80
2881 2882	CG	LEU		714	24.549		101.456		45.27
		LEU		714	23.237		102.419		45.36
2883 2884		LEU			25.513		103.031		43.80
4004	CDZ	טמע	D	/ I 4	45.513	10.577	102.333	1.00	13.00

FIGURE 3BF

A	В	С	D	E	F	G	Н	I	J
2885	С	LEU	В	714	26.436	8.393	99.951	1.00	40.57
2886	0	LEU		714	27.671	8.526	100.117	1.00	40.01
2887	N	GLN		715	25.900	7.402	99.314		40.78
2888	CA	GLN		715	26.755	6.362	98.870	1.00	40.81
2889	CB	GLN		715	25.933	5.288	98.183		40.42
2890	CG	GLN		715	25.177	4.515	99.255		40.01
2891	CD	GLN		715	24.070	3.635	98.723		44.67
2892	OE1	GLN		715	23.548	3.831	97.622		44.92
2893	NE2	GLN	В	715	23.716	2.651	99.517		48.08
2894	С	GLN		715	27.860	6.935	98.036		39.80
2895	0	GLN		715	29.054	6.675	98.339		42.92
2896	N	LEU		716	27.532	7.760	97.064	1.00	36.73
2897	CA	LEU		716	28.556	8.274	96.227		35.84
2898	CB	LEU		716	27.903	9.036	95.104	1.00	37.36
2899	CG	LEU		716	27.084	8.148	94.217	1.00	36.58
2900	CD1	LEU		716	26.356	9.177	93.311	1.00	
2901		LEU		716	27.996	7.350	93.371	1.00	
2902	C	LEU		716	29.573	9.163	96.975	1.00	36.89
2903	0	LEU		716	30.819	9.095	96.782	1.00	
2904	N	VAL		717	29.051	10.026	97.831		37.35
2905	CA	VAL	В	717	29:898	10.905	98.613	1.00	36.10
2906	CB	VAL		717	28.967	11.708	99.387	1.00	37.20
2907	CG1	VAL		717	29.667	12.776	100.344	1.00	33.48
2908	CG2	VAL		717	28.088	12.401	98.375	1.00	38.82
2909	C	VAL	В	717	30.870	10.002	99.410	1.00	38.05
2910	0	VAL		717	32.154	10.206	99.454	1.00	37.55
2911	N	GLY	В	718	30.264	8.952	99.981	1.00	36.80
2912	CA	GLY	В	718	31.042	8.022	100.772	1.00	33.97
2913	C	GLY	В	718	32.163	7.457	100.020	1.00	34.81
2914 -	0	GLY	В	718	33.349	7.436	100.512	1.00	37.01
2915	N	MET	В	719	31.892	7.099	98.779	1.00	34.31
2916	CA	MET	В	719	33.019	6.609	97.959	1.00	31.67
2917	CB	MET	В	719	32.491	6.176	96.577	1.00	32.74
2918	CG	MET	В	719	31.662	4.841	96.825	1.00	35.62
2919	SD	MET	В	719	30.875	4.103	95.295	1.00	55.32
2920	CE	MET	В	719	30.945	5.495	94.494	1.00	42.34
2921	C		В	719	34.081	7.610	97.784		30.03
2922	0	MET	В	719	35.279	7.293	97.765		32.08
2923	N	LEU	В	720	33.687	8.847	97.618		30.17
2924	CA	LEU	В	720	34.667	9.890	97.346		33.37
2925	CB	LEU	В	720	33.986	11.242	96.935		32.33
2926	CG	LEU		720	33.343	11.032	95.575		38.69
2927	CD1	LEU	В	720	32.375	12.150	95.300	1.00	38.75
2928	CD2	LEU		720	34.427	10.867	94.495		35.80
2929	C	LEU		720	35.489	10.109	98.597		32.85
2930	0	LEU		720	36. <i>6</i> 71	10.336	98.518		31.06
2931	N	ARG		721	34.809	10.018	99.755		34.48
2932	CA	ARG		721	35.496		100.996		33.62
2933	CB	ARG		721	34.472		102.146		35.11
2934	CG	ARG		721	35.051		103.478		34.63
2935	CD	ARG		721	35.575		104.326		39.88
2936	NE	ARG	В	721	36.004	9.899	105.636	1.00	43.02

FIGURE 3BG

A	В	C	D	E	F	G	Н	I	J
2937	CZ	ARG	B	721	36.937	9.323	106.397	1.00	45.17
2938		ARG		721	37.612		105.961		40.58
2939		ARG		721	37.213	9.851	107.611	1.00	38.32
2940	C	ARG		721	36.678	9.202	101.170	1.00	31.,50
2941	0	ARG		721	37.783		101.591	1.00	
2942	N	GLY		722	36.429	7.940	100.919	1.00	
2943	CA	GLY	В	722	37.450	6.885	100.918	1.00	24.89
2944	С	GLY		722	38.535	7.253	99.976	1.00	26.45
2945	0	GLY	В	722	39.751	7.161	100.307	1.00	27.04
2946	N	ILE	В	723	38.180	7.638	98.764	1.00	24.68
2947	CA	ILE	В	723	39.285	7.928	97.861	1.00	25.69
2948	CB	ILE	В	723	38.728	8.341	96.509	1.00	25.40
2949	CG1	ILE	В	723	38.089	7.129	95.744	1.00	23.38
2950	CD1	ILE	В	723	36.956	7.550	94.656	1.00	17.00
2951	CG2	ILE	В	723	39.915	8.818	95.562	1.00	25.42
2952	С	ILE	В	723	40.040	9.056	98.437	1.00	27.97
2953	0	ILE	В	723	41.273	9.063	98.412	1.00	29.92
2954	N	ALA	В	724	39.321	10.112	98.878	1.00	27.72
2955	CA	ALA	В	724	40.055	11.203	99.382	1.00	31.14
2956	CB	ALA	В	724	39.092	12.388	99.837		30.09
2957	C	ALA	В	724	40.994	10.756	100.578	1.00	32.43
2958	0	ALA		724	42.102	11.293	100.707	1.00	36.23
2959	N	ALA	В	725	40.599	9.778	101.386	1.00	
2960	CA	ALA		725	41.367	9.437		1.00	
2961	CB	ALA		725	40.465	8.568	103.649	1.00	
2962	C	ALA		725	42.563	8.658	102.180		33.06
2963	0	ALA		725	43.630		102.838		36.69
2964	N	GLY		726	42.407	7.837			29.85
2965	CA	GLY		726	43.519	7.036	100.688		26.93
2966	C	GLY		726	44.531		100.151		31.48
2967	0	GLY		726	45.699		100.370	1.00	
2968	N	MET		727	44.033	9.136	99.451	1.00	
2969	CA	MET		727	44.899	10.121	98.846	1.00	
2970	CB		В	727	44.051	10.999	97.853	1.00	
2971	CG		В	727	43.815	10.423	96.365	1.00	31.54
2972	SD		В	727 727	45.180	9.612	95.806 95.492		35.66 31.92
2973	CE	MET MET			46.441 45.618	10.934	100.018		33.03
2974	C				46.780	11.331	99.892		31.10
2975	O N			727	44.889		101.078		33.25
2976 2977	N CA			728 728	45.494		102.185		35.83
	CB			728	44.516		102.103		36.03
2978 2979	CG			728	45.095		103.204		41.39
2979	CD			728	44.169		105.549		49.57
2980	CE			728	44.504		106.868		58.31
2981	NZ			728	44.561		100.888		63.45
2983	C			728	46.658		107.388		38.33
2984	0			728	47.792		102.743		39.63
2985	N	TYR		729	46.494		103.003		36.94
2986	CA			729	47.452		102.017		36.82
2987	CB			729	46.858		103.213		34.05
2988	CG			729	47.899		103.835		34.37
2,00			_		17.000	5.557			

FIGURE 3BH

A	В	С	D	E	F	G	Н	I	J
2989	CD1	TYR	В	729	48.409	6.323	105.122	1.00	31.09
2990	CE1	TYR	В	729	49.368	5.343	105.286	1.00	25.86
2991	CZ	TYR		729	49.864	4.733	104.160	1.00	32.58
2992	OH	TYR	В	729	50.764	3.772	104.302	1.00	30.28
2993	CE2	TYR		729	49.369	5.022	102.863	1.00	28.90
2994	CD2	TYR		729	48.343	5.918	102.735	1.00	28.62
2995	C	TYR		729	48.625	9.040	102.348	1.00	38.24
2996	0	TYR		729	49.760	9.011	102.837	1.00	
2997	N	LEU		730	48.419	9.012	101.057	1.00	37.36
2998	CA	LEU		730	49.598	8.971	100.182	1.00	38.39
2999	CB	LEU	В	730	49.161	8.801	98.691	1.00	38.07
3000	CG	LEU	В	730	49.096	7.274	98.506	1.00	40.77
3001	CD1	LEU	В	730	48.033	6.879	97.535	1.00	46.74
3002	CD2	LEU	В	730	50.540	6.625	98.141	1.00	40.15
3003	C	LEU	В	730	50.415	10.239	100.271	1.00	36.79
3004	0	LEU	В	730	51.565	10.238	100.325	1.00	35.87
3005	N	ALA	В	731	49.753	11.330	100.211	1.00	38.07
3006	CA	ALA	В	731	50.421	12.597	100.382	1.00	41.33
3007	CB	ALA	В	731	49.377	13.802	100.342	1.00	35.88
3008	C	ALA	В	731	51.191	12.559	101.743	1.00	41.93
3009	0	ALA	В	731	52.353	12.861	101.784	1.00	41.92
3010	N	ASN	В	732	50.556	12.176	102.837	1.00	43.62
3011	CA	ASN	В	732	51.340	12.240	104.035	1.00	45.24
3012	CB	ASN	В	732	50.558	11.897	105.275	1.00	45.55
3013	CG	ASN	В	732	49.605	12.947	105.613	1.00	45.67
3014	OD1	ASN	В	732	49.792	14.047	105.114	1.00	45.78
3015	ND2	ASN	В	732	48.503	12.620	106.390	1.00	42.26
3016	C	ASN	В	732	52.439	11.247	103.945	1.00	46.19
3017	0	ASN	В	732	53.250	11.259	104.809	1.00	48.18
3018	N	MET	В	733	52.475	10.319	102.986		45.55
3019	CA	MET	В	733	53.611	9.396	102.967		42.71
3020	CB	MET	В	733	53.181	8.051	102.457		43.29
3021	CG	MET	В	733	52.418	7.229			44.11
3022	SD	MET	В	733	53.390	6.662	104.809	1.00	45.37
3023	CE	MET	В	733	54.537	5.722	104.067		
3024	C	MET	В	733	54.473	10.030	101.973		43.07
3025	0	MET		733	55.449	9.447	101.489		39.67
3026	N	ASN			54.114		101.639		45.47
3027	CA			734	54.895		100.620		45.76
3028	CB			734	56.293		101.146		48.02
3029	CG	ASN			56.917		100.855		55.08
,3030		ASN		734	57.998		100.227		57.65
3031		ASN			56.191		101.227		57.16
3032	C	ASN		734	55.017	11.329	99.233		44.84
3033	0	ASN		734	56.122	11.359			45.91
3034	N G7	TYR		735	53.933	10.733	98.723		43.14
3035	CA	TYR		735	53.846	10.348	97.298		39.99
3036	CB	TYR		735	53.511	8.904	97.196		42.06
3037	CG	TYR		735	54.612	7.939	97.303		39.82
3038	CD1	TYR		735	55.073	7.272	96.195		40.71
3039		TYR			56.143	6.364	96.327		49.17 49.26
3040	CZ	TYR	В	735	56.659	6.076	97.610	1.00	43.20

FIGURE 3BI

Α	В	C	D	E	F	,	G		Н	I	J
3041	ОН	TYR	B	735	57.6	81 5	.174	97.	808	1.00	53.69
3042	CE2	TYR		735	56.1		.710		706		46.44
3043	CD2	TYR		735	55.1		.596		563		44.21
3044	C	TYR		735	52.7		.131		513		40.01
3045	Ō	TYR		735	51.6		.403		063		38.30
3046	N	VAL		736	53.0		.534		242	1.00	39.05
3047	CA	VAL		736	52.1	.55 12	.135		317	1.00	37.57
3048	СВ	VAL	В	736	52.9		.826	93.	220		40.62
3049	CG1			736	52.2	10 13	.815	92.	384	1.00	40.34
3050	CG2	VAL	В	736	54.1	.64 13	.336	93.	780	1.00	46.41
3051	C	VAL	В	736	51.8	24 10	.887	93.	435	1.00	37.17
3052	0	VAL	В	736	52.7	35 10	.241	92.	930	1.00	29.75
3053	N	HIS	В	737	50.5	39 10	.633	93.	185	1.00	37.35
3054	CA	HIS	В	737	50.1	.06 9	.466	92.	371	1.00	37.48
3055	CB	HIS	В	737	48.6	45 9	.217	92.	703	1.00	37.46
3056	CG	HIS	В	737	48.1	.49 7	.922		212		38.36
3057	ND1	HIS	В	737	47.7	788 7	.709		894		33.89
3058	CE1			737	47.4		.446		753		38.45
3059	NE2	HIS		737	47.5		.845		941		38.58
3060		HIS		737	48.0		.737		850		36.23
3061	C			737	50.3		.689		885		37.35
3062	0	HIS		737	50.9		.930		179		37.49
3063	N	ARG		738	49.9		.862		420	1.00	
3064	CA	ARG		738	50.1		.215		025		41.82
3065	CB	ARG		738	51.5		.752		576		42.45
3066	CG	ARG		738	52.9		.362		171		43.81
3067	CD	ARG		738	53.9		.099		306		50.41
3068	NE	ARG		738	54.4		.640		014		59.49 66.23
3069	CZ	ARG		738	55.0		.452		751 671		66.49
3070 3071	NH1	ARG ARG		738 738	55.1 55.5		.499 .202		535		66.53
3071	C	ARG		738	49.0		.581		104		42.10
3072	0	ARG		738	48.8		.056		025		42.38
3074	N	ASP		739	48.3		.578		572		40.65
3075	CA	ASP		739	47.4		.839		683		37.25
3076	CB	ASP		739	48.0		.585		132		36.50
3077	CG	ASP		739	47.4		.043		859		39.77
3078		ASP			46.7		.845	85.	259		35.07
3079		ASP			47.5		.843		423		38.97
3080	C	ASP		739			.470	88.	383	1.00	33.96
3081	0	ASP	В	739	45.6	41 7	.385	88.	230	1.00	33.13
3082	N	LEU	В	740	45.6	12 9	.440	89.	054	1.00	32.76
3083	CA	LEU	В	740	44.3	85 9	.304	89.	792	1.00	32.28
3084	CB	LEU	В	740	44.2	18 10	.378	90.	903	1.00	28.90
3085	CG	LEU	В	740	42.9		.273		633	1.00	31.41
3086	CD1	LEU	В	740	42.7		.844		335		29.24
3087	CD2	LEU	В	740	42.7		.301	92.	751		31.09
3088	C	LEU	В	740	43.2		.487		854		33.40
3089	0	LEU			42.9		.631		367		32.41
3090	N	ALA			42.3		.464		851		32.10
3091	CA	ALA				56 8			939		31.90
3092	CB .	ALA	В	741	41.7	95 8	.228	86.	47 3	1.00	25.99

FIGURE 3BJ

A	В	C	D	E	F	G	Н	I	J
3093	C	ALA		741	40.361	7.405	88.402		30.39
3094	0	ALA		741	40.849	6.468	89.090		32.43
3095	N	ALA		742	39.091	7.450	87.997		30.00
3096	CA	ALA		742	38.230	6.405	88.434		28.92
3097	CB	ALA		742	36.771	6.688	88.146		32.43
3098	C	ALA		742	38.702	5.046	87.904		31.77
3099	0	ALA		742	38.551	4.078	88.607		30.25
3100	N	ARG		743	39.282	4.907	86.696		31.71
3101	CA	ARG		743	39.685	3.568	86.348		32.57
3102	CB	ARG		743	40.311	3.530	84.893		30.75
3103	CG	ARG		743	41.249	4.519	84.625		29.61
3104	CD			743	42.260	4.076	83.465		43.52
3105	NE	ARG		743	43.297	5.113	83.400		45.54
3106	CZ	ARG		743	42.950	6.342	83.147		45.33
3107		ARG		743	41.651	6.558	82.868		38.16
3108		ARG		743	43.844	7.305	83.199	1.00	
3109	C	ARG		743	40.697	3.045	87.291	1.00	
3110	0	ARG		743	41.122	1.917	87.211		33.13
3111	N	ASN		744	41.306	3.909	88.055		33.51
3112	CA	ASN		744	42.357	3.337	88.857		32.87
.3113	CB	ASN		744	43.651	4.144	88.701		33.36
3114	CG			744	44.393	3.813	87.400		34.78
3115				744	44.062	2.792	86.820		48.21
3116				744	45.248	4.718	86.851		31.64
3117	C	ASN		744	41.888	3.251	90.300		34.12
3118	0	ASN		744	42.689	3.242	91.157		36.14
3119	N	ILE		745	40.592	3.314	90.558		32.33
3120	CA	ILE		745	40.098	3.112	91.861		31.92
3121	CB	ILE		745	39.154	4.230	92.239		31.00
3122	CG1	ILE		745	39.824	5.704	92.215		32.78
3123	CD1	ILE		745	41.204	5.701	92.993	1.00	32.89
3124	CG2		В	745	38.602	3.943	93.507	1.00	
3125	C	ILE		745	39.347	1.767	91.809	1.00	
3126	0	ILE		745	38.592	1.602	90.864		32.62
3127	N	LEU		746	39.593	0.833	92.752		29.93
3128	CA	LEU		746	38.994	-0.526	92.790		28.79 27.96
3129	CB	LEU		746	40.047	-1.578 -1.793	93.158 92.142	1.00	27.80
3130	CG		В	746	41.188				36.80
3131		LEU			42.431	-2.746	92.482		32.27
3132		LEU		746	40.582	-2.251	90.857		
3133	C	LEU		746	37.941	-0.457	93.907		31.64 32.71
3134	0	LEU			38.176	0.242	94.933		
3135	N	VAL			36.752	-1.061	93.727		32.95 33.60
3136	CA	VAL			35.729	-0.956	94.751		35.06
3137	CB			747	34.337	-0.627	94.211		32.73
3138		LAV			33.569	0.153	95.190 92.802		36.08
3139		VAL		747	34.311	-0.145			32.18
3140	C	VAL		747	35.379	-2.348	95.139		32.10
3141	0	VAL			35.438	-3.132	94.271		32.47
3142	N Ca	ASN			34.809	-2.569	96.331		32.11
3143	CA			748	34.300	-3.873	96.670		29.71
3144	CB	NCA	B	748	35.076	-4.503	97.805	1.00	27.11

FIGURE 3BK

A	В	С	D	E	F	G	Н	I	J
3145	CG	ASN	В	748	34.872	-3.789	99.093	1.00	30.19
3146		ASN		748	34.002	-2.965	99.154		29.21
3147		ASN		748	35.724	-4.051	100.145		27.55
3148	C	ASN		748	32.782	-3.847	96.880		32.91
3149	0	ASN	В	748	32.137	-2.821	96.558	1.00	34.46
3150	N	SER	В	749	32.200	-4.931	97.392	1.00	31.86
3151	CA	SER	В	749	30.779	-4.924	97.589	1.00	32.16
3152	CB	SER	В	749	30.203	-6.341	97.762	1.00	33.15
3153	OG	SER	В	749	30.792	-7.147	98.772	1.00	33.73
3154	C	SER	В	749	30.390	-4.108	98.724	1.00	33.33
3155	0	SER	В	749	29.213	-3.877		1.00	31.39
3156	N	ASN	В	750	31.368	-3.666	99.517	1.00	34.87
3157	CA	ASN	В	750	30.972	-2.694	100.547		35.09
3158	CB	ASN	В	750	31.781	-2.859	101.809		37.06
3159	CG	ASN	В	750	31.421		102.582		41.91
3160		ASN		750	30.278		102.549		38.82
3161	ND2	ASN	В	750	32.424		103.275		46.14
3162	C	ASN		750	31.082	-1.295	100.025		34.62
3163	0	ASN		750	30.760		100.737		36.26
3164	N	LEU		751	31.385	-1.151	98.738		31.97
3165	ÇA	LEU		751	31.511	0.150	98.134		33.21
3166	CB	LEU		751	30.275	1.085	98.379		33.30
3167	CG	LEU		751	28.944	0.583	97.933		29.08
3168		LEU		751	27.770	1.538	97.936		34.22
3169	CD2			751	29.187	0.432	96.569		25.04
3170	C	LEU		751	32.774	0.820	98.675		31.97
3171	0	LEU		751	32.932	1.949	98.482		32.37
3172	N	VAL		752	33.673	0.112	99.330		31.80
3173	CA			752	34.884	0.756	99.838		32.23
3174	CB	VAL		752	35.557		100.847		34.25
3175		VAL		752	36.916	0.159	101.117		28.08
3176	CG2	VAL		752	34.701		102.072		27.86
3177	C	VAL		752	35.761	0.974	98.604		34.48
3178	0	VAL		752	35.900	0.035	97.753		33.89
3179	N	CYS		753	36.345	2.183	98.450		34.53
3180	CA	CYS CYS		753	37.139 36.667	2.463 3.795	97.238 96.590		33.46 32.57
3181	CB	CYS		753	35.024	3.795			33.85
3182 3183	SG C	CYS			38.595	2.504	97.641		32.87
3184	0			753	38.918				33.65
3185	N			754	39.490	2.019			31.25
3186	CA			754	40.879	2.069			28.59
3187	CB	LYS			41.393	0.682	97.601		28.62
3188	CG	LYS			40.612	0.002	98.777		25.26
3189	CD	LYS			41.255	-1.359	99.092		26.47
3190	·CE	LYS			40.451		100.084		31.42
3191	NZ	LYS			41.028		101.467		36.53
3192	C	LYS			41.659	2.488	95.931		29.63
3193	0	LYS			41.451	1.951	94.764		29.44
3194	N	VAL			42.643		96.190		28.68
3195	CA	VAL			43.512		95.158		30.76
3196	CB	VAL			44.484	4.852	95.681		29.87
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FIGURE 3BL

Α .	В	С	D	E	F	G	Н	I	J
3197	CG1	VAL	В	755	45.380	5.460	94.520	1.00	26.20
3198	CG2	VAL			43.750	5.907	96.257		28.72
3199	C			755	44.391	2.708	94.759		31.83
3200	0			755	44.894	2.059	95.618		30.86
3201	N			756	44.722	2.641	93.486		33.08
3202	CA			756	45.431	1.545	92.914		36.43
3203	CB			756	44.472	0.481	92.259		37.70
3204	OG			756	45.281	-0.617	91.571		40.69
3205	C	SER			46.368	2.061	91.849		37.72
3206	0			756	46.466	3.263	91.576		37.99
3207	N			757	46.978	1.130	91.147		38.48
3208	CA	ASP			47.861	1.499	90.074		41.72
3209	CB	ASP			47.023	1.917	88.88		41.39
3210	CG	ASP			47.849	1.913	87.574		50.91
3211		ASP			47.211	2.091	86.487		51.60
3212		ASP			49.141	1.757	87.558		52.69
3213	C	ASP		757	49.001	2.490	90.467		41.65
3214	0	ASP		757	48.943	3.671	90.267		41.11
3215	N	PHE		758	50.076	1.995	91.048		43.52
3216	CA			758	51.087	2.948	91.493		44.14
3217	CB			758	51.525	2.631	92.952		43.50
3218	CG	PHE			50.456	2.888	93.920		38.35
3219		PHE			50.308	4.177	94.499		33.03
3220		PHE			49.233	4.488	95.392		33.75
3221	CZ	PHE			48.282	3.458	95.734	1.00	35.68
3222		PHE		758	48.419	2.141	95.050	1.00	35.33
3223	CD2	PHE	В	758	49.531	1.901	94.184	1.00	37.29
3224	C	PHE	В	758	52.199	3.247	90.454	1.00	45.65
3225	0	PHE	В	758	53.160	4.088	90.646	1.00	46.52
3226	N	GLY	В	759	51.903	2.709	89.282	1.00	46.03
3227	CA	GLY	В	759	52.617	2.856	88.048	1.00	47.12
3228	C	GLY	В	759	53.353	4.173	87.857	1.00	50.02
3229	0	GLY	В	759	54.588	4.163	87.553	1.00	53.05
3230	N	LEU	В	760	52.664	5.294	87.911	1.00	46.21
3231	CA	LEU	В	760	53.371	6.532	87.683	1.00	47.41
3232	CB	LEU	В	760	52.504	7.502	86.833		46.97
3233	CG	LEU			52.025	7.054	85.450		52.65
3234		LEU			51.187				51.82
3235	CD2	LEU			53.252				51.03
3236	С			760	53.628				47.35
3237	0	LEU			53.755		88.928		47.23
3238	N	SER			53.643				48.54
3239	CA	SER			53.583	7.610	91.262		49.64
3240	CB	SER			52.674	7.066	92.329		47.14
3241	OG	SER			53.142	5.812	92.428		48.99
3242	C	SER			54.965	7.803	91.813		50.77
3243	0	SER			55.814	6.895	91.672		51.89
3244	N	ARG			55.227	8.947	92.427		50.64
3245	CA	ARG			56.576	9.132	92.940		51.02
3246	CB	ARG				9.689			52.96
3247	CG	ARG			57.051				55.70
3248	CD	ARG	В	762	57.559	10.114	89.374	1.00	67.92

FIGURE 3BM

A	В	С	D	E	F	G	Н	I	J
3249	NE	ARG	В	762	57.115	8.769	88.974	1.00	75.81
3250	CZ	ARG	В	762	57.530	8.088	87.860	1.00	79.84
3251		ARG		762	57.034	6.858	87.589	1.00	77.74
3252	NH2	ARG		762	58.432	8.624	87.030	1.00	79.01
3253	C	ARG		762	56.692	9.874	94.202	1.00	50.69
3254	0	ARG		762	55.762	10.587	94.600	1.00	
3255	N	VAL		763	57.834	9.667	94.879	1.00	
3256	CA	VAL		763	58.143	10.438	96.111		53.91
3257	CB	VAL		763	59.438	9.932	96.770		56.45
3258	CG1	VAL		763	59.822	10.769	98.058		53.41
3259	CG2	VAL		763	59.293	8.431	97.046		53.98
3260	C	VAL		763	58.323	11.921	95.757		52.61
3261	0	VAL		763	58.998	12.205	94.849		52.54
3262	N	ALA		764	57.680	12.818	96.460	1.00	
3263	CA	ALA		764	57.640	14.215	96.083	1.00	
3264	CB	ALA		764	56.842	15.013	97.079		55.95
3265	C	ALA		764	58.997	14.901	95.822	1.00	58.47
3266	o	ALA		764	60.011	14.667	96.486		58.95
3267	N	ALA		778	52.512	8.707	77.650		63.16
3268	CA	ALA		778	53.274	9.379	78.726		64.24
3269	CB	ALA		778	54.203	10.520	78.164		63.79
3270	C	ALA		778	52.320	9.882	79.851		63.12
3271	0	ALA		778	52.320	9.355	80.966		63.11
3272	N	ILE		779	51.472	10.863	79.572	1.00	61.82
3273	CA	ILE		779	50.565	11.342	80.639	1.00	59.71
3274	CB	ILE		779	51.075	12.717	81.033	1.00	60.71
3275	CG1	ILE		779	52.166	12.503	82.090	1.00	62.19
3276	CD1	ILE	В	779	53.432	13.193	81.727	1.00	66.21
3277	CG2	ILE	В	779	49.943	13.685	81.434	1.00	62.88
3278	C	ILE	В	779	49.010	11.248	80.435	1.00	57.07
3279	0	ILE	В	779	48.552	11.065	79.280	1.00	55.98
3280	N	PRO	В	780	48.228	11.201	81.549	1.00	54.65
3281	CA	PRO	В	780	46.770	11.559	81.509	1.00	52.75
3282	CB	PRO	В	780	46.321	11.448	82.969	1.00	53.47
3283	CG	PRO	В	780	47.247	10.442	83.543	1.00	51.28
3284	CD	PRO	В	780	48.603	10.801	82.915	1.00	54.55
3285	C	PRO	В	780	46.610	12.952	81.191	1.00	50.88
3286	0	PRO	В	780	46.988	13.770	82.008	1.00	56.60
3287	N	ILE	В	781	46.112	13.222	80.017	1.00	46.48
3288	CA	ILE	В	781	45.849	14.560	79.767	1.00	43.01
3289	CB	ILE	В	781	45.897	14.790	78.286	1.00	41.97
3290	CG1	ILE	В	781	47.316	15.269	78.013	1.00	45.31
3291	CD1	ILE	В	781	48.308	14.194	77.831	1.00	50.28
3292	CG2	ILE	В	781	45.107	15.941	77.979	1.00	38.03
3293	C	ILE	В	781	44.611	15.023	80.581	1.00	40.95
3294	0	ILE	В	781	44.748	15.814	81.489		40.34
3295	N	ARG	В	782	43.460	14.431	80.284	1.00	41.60
3296	CA	ARG	В	782	42.166	14.646	80.837		38.55
3297	CB	ARG	В	782	41.127	13.968	79.858		40.91
3298	CG	ARG	В	782	40.395	12.734	80.126		39.72
3299	CD	ARG	В	782	40.142	12.040	78.779		44.03
3300	NE	ARG	В	782	38.977	12.556	78.126	1.00	50.70

FIGURE 3BN

A	В	С	D	E	F	G	Н	I	J
3301	CZ	ARG		782	38.978	13.000	76.853		52.30
3302		ARG		782	37.828	13.451	76.324		46.70
3303		ARG		782	40.126	13.022	76.153	1.00	
3304	C	ARG		782	42.033	14.486	82.369		36.84
3305	0	ARG		782	41.124	15.127	82.932		37.92
3306	N	TRP		783	42.986	13.873	83.062		35.41
3307	CA	TRP		783	42.931	13.863	84.548		36.23
3308	CB	TRP		783	43.045	12.446	85.168		35.36
3309	CG	TRP		783	41.939	11.580	84.894		34.89
3310	CD1	TRP		783	40.959	11.347	85.728		34.55 35.15
3311	NE1	TRP TRP		783 783	40.032 40.417	10.518	85.152 83.889		28.35
3312	CE2 CD2	TRP		783	41.611	10.196 10.885	83.662		29.59
3313 3314	CE3	TRP		783	42.243	10.883	82.424		33.66
3315	CZ3	TRP		783	41.642	9.873	81.461		39.20
3316	CH2	TRP		783	40.386	9.270	81.697		30.32
3317	CZ2	TRP		783	39.750	9.394	82.892		26.79
3318	C	TRP		783	44.019	14.767	85.182		37.26
3319	0	TRP		783	44.078	14.934	86.462	1.00	32.75
3320	N	THR		784	44.868	15.335	84.294		38.13
3321	CA	THR		784	46.074	16.069	84.782	1.00	
3322	CB	THR		784	47.220	15.822	83.921		38.22
3323		THR		784	47.407	14.394	83.791		32.84
3324	CG2	THR		784	48.499	16.365	84.574		27.62
3325	C	THR		784	45.959	17.558	84.819		42.12
3326	0	THR		784	45.451	18.183	83.855		44.07
3327	N	ALA	В	785	46.415	18.118	85.944		42.78
3328	CA	ALA	В	785	46.490	19.525	86.209	1.00	42.20
3329	CB	ALA	В	785	47.126	19.714	87.503	1.00	41.73
3330	C	ALA	В	785	47.330	20.250	85.152	1.00	42.59
3331	0	ALA	В	785	48.358	19.707	84.633	1.00	41.88
3332	N	PRO	В	786	46.867	21.443	84.823	1.00	41.88
3333	CA	PRO	В	786	47.509	22.281	83.783	1.00	43.28
3334	CB	PRO	В	786	46.514	23.437	83.610		42.82
3335	CG	PRO	В	786	45.682	23.472	84.854		
3336	CD	PRO		786	45.625	22.022	85.316		40.34
3337	С	PRO		786	48.937	22.647	84.199		44.36
3338	0			786	49.876	22.335	83.415		43.75
3339	N			787	49.161		85.458		47.66
3340	CA			787	50.585				48.56
3341	CB			787	50.799	23.521	87.366		50.25
3342	CG			787	50.506	22.415	88.438		47.77
3343	CD			787	49.055	22.343	88.835		45.14
3344		GLU			48.239	23.053	88.217		47.89
3345		GLU		787	48.675	21.581	89.750		48.40
3346	C	GLU			51.413	22.011	85.524		48.85
3347	0	GLU			52.601	22.103	85.448		49.02
3348	N	ALA			50.810	20.871	85.240		50.59
3349	CA	ALA			51.630	19.703	85.119		52.43
3350	CB	ALA			51.138	18.650			53.63
3351	C			788	51.881				54.39
3352	0	ALA	R	788	52.825	18.429	83.538	1.00	53.44

FIGURE 3BO

A	В	С	D	E	F	G	Н	I	J
3353	N.	ILE	В	789	51.076	19.709	82.848	1.00	58.49
3354	CA	ILE	В	789	51.180	19.309	81.466	1.00	60.06
3355	СВ	ILE	В	789	49.791	19.422	80.879	1.00	60.19
3356	CG1	ILE	В	789	49.005	18.288	81.542	1.00	57.40
3357	CD1	ILE	В	789	47.545	18.338	81.498	1.00	52.54
3358	CG2		В	789	49.888	19.223	79.405	1.00	60.76
3359	С		В	789	52.175	20.260	80.860	1.00	61.11
3360	0		В	789	53.217	19.903	80.277	1.00	61.28
3361	N	SER		790	51.775	21.498	81.090	1.00	63.37
3362	CA	SER	В	790	52.455	22.746	80.870	1.00	65.13
3363	CB	SER	В	790	51.887	23.687	81.908	1.00	64.75
3364	OG	SER	В	790	52.132	22.945	83.109	1.00	72.95
3365	С	SER	В	790	53.883	22.498	81.324	1.00	65.49
3366	0	SER		790	54.721	22.181	80.519	1.00	65.88
3367	N	TYR		791	54.080	22.534	82.650	1.00	67.60
3368	CA	TYR	В	791	55.356	22.655	83.371	1.00	67.61
3369	CB	TYR	В	791	55.133	23.658	84.492	1.00	67.72
3370	CG	TYR	В	791	54.527	24.979	84.072	1.00	69.06
3371	CD1	TYR	В	791	53.373	25.468	84.681	1.00	73.54
3372	CE1	TYR	В	791	52.811	26.729	84.343	1.00	77.27
3373	CZ	TYR	В	791	53.434	27.536	83.361	1.00	78.11
3374	OH	TYR	В	791	52.888	28.779	83.031	1.00	74.15
3375	CE2	TYR	В	791	54.617	27.080	82.777	1.00	76.67
3376	CD2	TYR	В	791	55.167	25.794	83.142	1.00	74.63
3377	С	TYR	В	791	55.841	21.341	83.987	1.00	67.44
3378	0	TYR	В	791	56.991	21.177	84.471	1.00	
3379	N	ARG	В	792	54.955	20.377	83.993	1.00	66.21
3380	CA	ARG	В	792	55.418	19.098	84.530		65.39
3381	CB	ARG	В	792	56.655	18.642	83.811		65.99
3382	CG	ARG		792	56.702	17.131	83.750	1.00	72.90
3383	CD	ARG		792	57.978	16.532	83.158	1.00	81.61
3384	NE	ARG		792	58.984	17.572	83.010	1.00	
3385	CZ	ARG		792	60.191	17.394	82.478	1.00	91.91
3386	NH1	ARG		792	60.980	18.468	82.408	1.00	
3387	NH2	ARG		792	60.592	16.196	82.009	1.00	
3388	C	ARG		792	55.624	19.127	86.033	1.00	61.73
3389	0	ARG		792	56.452	18.430	86.557		61.41 58.85
3390	N			793	54.792		86.722		
3391	CA			793	54.853	20.039	88.179		56.36
3392	CB			793	54.957	21.543	88.590		55.91
3393	C			793	53.713	19.275	88.952		55.37 53.05
3394	0			793	52.576	19.774	89.157		53.03
3395	N			794	54.087 53.197	18.085	89.403 90.066		52.23
3396	CA			794	53.197	17.141 15.682	89.718		51.93
3397	CB			794 794	53.400	15.338	88.275		52.20
3398	CG				52.102	15.265	87.761		55.84
3399		PHE		794	51.857	14.993	86.368		57.33
3400 3401	CE1 CZ	PHE PHE		794	52.972	14.849	85.527		57.10
3401	CE2	PHE		794 794	54.271	14.849	86.076		51.98
3402		PHE			54.461	15.189			50.42
3403	CDZ			79 4	53.311	17.374	91.542		50.46
3404	C	rne	٥	194	JJ.JII	11.3/4	J1.J42	1.00	50.10

FIGURE 3BP

A	В	С	D	E		F	(3		Н	I	J
3405	0	PHE	В	794	54	.347	17.4	125	92.	050	1.00	51.33
3406	N	THR		795		.221	17.3			249		49.78
3407	CA	THR		795		. 232	17.8			561		47.81
3408	CB	THR		795		.007	19.2			227		48.89
3409	OG1	THR		795		.044	20.0			792	1.00	53.29
3410	CG2	THR		795		.667	19.8			729		46.81
3411	C	THR		795		. 983	17.2			222		46.44
3412	Ö	THR		795		.005	16.9			564	1.00	
3413	N	SER		796		.946	17.0			504		42.66
3414	CA	SER		796		.646	16.7			943		42.64
3415	CB	SER		796		.536	16.6			500		42.15
3416	OG	SER		796		.321	15.5	565		792		41.91
3417	C	SER		796		.526	17.5			328		41.72
3418	Ō	SER		796		.377	17.0			157	1.00	41.30
3419	N	ALA		797		.784	18.8			079	1.00	40.89
3420	CA	ALA		797		. 663	19.6		94.	615	1.00	40.50
3421	СВ	ALA	В	797		.022	21.3			671	1.00	39.74
3422	C	ALA	В	797		.280	19.3	305	93.	173	1.00	39.17
3423	0	ALA	В	797	46	.128	19.5	595	92.	751	1.00	38.84
3424	N	SER	В	798	48	.263	18.7		92.	489	1.00	34.53
3425	CA	SER	В	798	48	. 225	18.0	096	91.	130	1.00	37.20
3426	CB	SER	В	798	49	.628	17.5	544	91.	024	1.00	36.03
3427	OG	SER	В	798	50	.147	17.3	397	89.	784	1.00	39.62
3428	C	SER	В	798	47	.230	16.9	905	91.	257	1.00	37.26
3429	0	SER	В	798	46	. 155	16.8	360	90.	659	1.00	39.61
3430	N	ASP	В	799	47	.482	16.0	337		210	1.00	38.19
3431	CA	ASP	В	799		.573	14.9	920	92.	473		37.01
3432	CB	ASP	В	799	47	.107	14.0	77	93.	579		35.52
3433	CG	ASP	В	799	48	.139	13.3	180		147		34.06
3434			В	799		.373	13.0			930		35.46
3435		ASP		799	48	.888	12.6			969		38.80
3436	C	ASP		799		.199	15.4			855		35.89
3437	0	ASP		799		.175	14.			609	1.00	
3438	N	VAL		800		.142	16.6			477		35.26
3439	CA			800		.822	17.			947		32.94
3440	CB			800		.940	18.2			019		34.11
3441		VAL				.646	19.1			117		22.48
3442		VAL				.469		599		515		28.48
3443	C			800		.950	17.5			768		34.34
3444	0			800	-	.709	17.4			760		35.47
3445	N			801		.636		049		764		34.34
3446	CA			801		.044		275		477		35.48 35.00
3447	CB			801		.091	18.9			507		
3448	CG CD1			801		.459 .141	19.1 18.2			157 174		40.40 38.90
3449		TRP TRP				.553	18.8			133		39.62
3450 3451	CE2	TRP				. 424	20.2			419		34.39
3452		TRP				.007	20.4			642		34.20
3453		TRP				.007	21.			138		38.91
3454	CZ3					. 445	22.			399		36.57
3455	CH2					. 952	22.4			152		36.98
3456	CZ2			801		. 885	21.2			652		38.72

FIGURE 3BQ

A	В	С	D	E	F	G	Н	I	J
3457	С	TRP	В	801	42.351	16.959	89.962	1.00	33.13
3458	0			801	41.094	16.871	89.763	1.00	32.82
3459	N			802	43.167	15.932	89.804	1.00	33.07
3460	CA			802	42.670	14.644	89.377	1.00	30.99
3461	CB			802	43.764	13.696	89.596	1.00	32.92
3462	OG			802	44.915	13.966	88.873	1.00	
3463	C			802	41.511	14.199	90.191		32.70
3464	0			802	40.470	13.693	89.697		33.27
3465	N			803	41.612	14.494	91.467		30.29
3466	CA			803	40.592	14.026	92.333		29.47
3467	CB			803	40.976	14.324	93.828		27.73
3468	CG			803	39.873	14.000	94.769		29.18
3469	CD1			803	39.025	15.007	95.261		23.67
3470	CE1			803	38.016	14.683	96.177		32.92
3471	CZ			803	37.764	13.282	96.514		31.89
3472	CE2	PHE			38.619	12.258	95.929		28.18
3473	CD2			803	39.656	12.633	95.129	1.00	
3474	C			803	39.283	14.713	92.014	1.00	
3475	0			803	38.185	14.221	92.288	1.00	
3476	N			804	39.385	15.925	91.508		31.66
3477	CA			804	38.192	16.682	91.178		32.09
3478	C			804	37.595	15.997	89.930		31.91
3479	0			804	36.344	15.792	89.811		32.78
3480	N			805	38.471	15.468	89.086		31.21
3481	CA			805	37.922	14.809	87.937	1.00	
3482	CB			805	39.019	14.336	86.958		31.83
3483	CG1			805	39.901	15.503	86.501		29.56
3484	CD1			805	39.060	16.699	85.638		28.04
3485	CG2			805	38.273	13.590	85.789		30.62
3486	C			805	37.187	13.531	88.399		30.39
3487	0			805	36.137	13.167	87.862		30.88
3488	N			806	37.856	12.771	89.253		30.81
3489	CA			806	37.335	11.519	89.853		28.37
3490	CB			806	38.295	10.897	90.978		29.63
3491		VAL			37.674	9.730	91.601		21.00
3492	CG2			806	39.518	10.536	90.425		22.65
3493	C			806	36.055	11.924	90.505		29.32
3494	0	VAL	В	806	35.066	11.258	90.312	1.00	32.00
3495	N			807	36.006	12.981	91.282		28.61
3496	CA			807	34.635	13.320	91.782	1.00	30.01
3497	CB			807	34.544	14.686	92.556	1.00	27.73
3498	CG			807	35.490	14.830	93.746		29.47
3499	SD			807	35.350	16.540	94.517	1.00	35.02
3500	CE			807	33.929	16.536	95.089	1.00	33.26
3501	C			807	33.615	13.403	90.606	1.00	30.22
3502	0			807	32.442	13.037	90.717	1.00	30.29
3503	N			808	34.040	13.980	89.473		31.44
3504	CA			808	33.026	14.215	88.453	1.00	28.58
3505	CB			808	33.626	15.123	87.374	1.00	30.92
3506	CG			808	32.681	15.593	86.292	1.00	26.01
3507	CD1			808	31.826	16.670	86.368	1.00	25.96
3508	NE1			808	31.178	16.794	85.186	1.00	34.62

FIGURE 3BR

A	В	С	D	E	F	G	Н	I	J
3509	CE2	TRP	В	808	31.566	15.779	84.355	1.00	32.11
3510	CD2	TRP			32.468	14.980	85.061		28.97
3511	CE3	TRP		808	33.064	13.909	84.398		28.52
3512	CZ3	TRP		808	32.709	13.687	83.032	1.00	32.24
3513	CH2	TRP		808	31.725	14.446	82.425	1.00	
3514	CZ2	TRP		808	31.185	15.521	83.050	1.00	
3515	C	TRP		808	32.712	12.873	87.869	1.00	28.00
3516	0	TRP			31.577	12.568	87.668	1.00	31.29
3517	N			809	33.684	12.013	87.650		27.30
3518	CA	GLU	В	809	33.330	10.714	87.110	1.00	28.51
3519	CB	GLU	В	809	34.555	9.884	86.910	1.00	30.85
3520	CG	GLU	В	809	35.617	10.432	86.024	1.00	25.12
3521	CD	GLU	В	809	36.813	9.571	86.014	1.00	28.19
3522	OE1	GLU	В	809	36.849	8.704	85.133	1.00	32.40
3523	OE2	GLU	В	809	37.778	9.798	86.791	1.00	31.60
3524	C	GLU	В	809	32.435	9.919	88.019	1.00	30.07
3525	0	GLU	В	809	31.575	9.111	87.555	1.00	33.66
3526	N	VAL	В	810	32.507	10.201	89.289	1.00	30.06
3527	CA	VAL	В	810	31.716	9.434	90.205	1.00	29.76
3528	CB	VAL	В	810	32.255	9.428	91.665	1.00	30.24
3529	CG1	VAL	В	810	31.095	9.097	92.609	1.00	24.88
3530	CG2	VAL	В	810	33.391	8.481	91.834	1.00	25.13
3531	C	VAL	В	810	30.346	10.058	90.287	1.00	
3532	0	VAL	В	810	29.381	9.349	90.313	1.00	27.09
3533	N	MET	В	811	30.247	11.393	90.308		32.39
3534	CA	MET	В	811	28.889	11.928	90.411		34.71
3535	CB			811	28.900	13.402	90.899		35.87
3536	CG	MET			29.590	13.624	92.224		38.06
3537	SD	MET			28.965	12.583	93.435		43.12
3538	CE	MET			27.111	12.868	93.575		35.71
3539	C	MET			28.162	11.746	89.043		33.74
3540	0	MET			27.022	11.928	88.905		36.24
3541	N			812	28.845	11.231	88.066		35.66
3542	CA			812	28.304	11.132	86.752		35.64
3543	CB	THR		812	29.319	11.867	85.953		37.45
3544	OG1	THR		812	28.697	12.834	85.169	1.00	
3545	CG2			812	30.251	11.113	85.174		23.27
3546				812	28.173	9.753	86.352		37.54
3547	0			812	27.786		85.230		38.76
3548	N			813	28.448	8.869			37.57
3549	CA			813	28.363		86.943		34.78
3550	CB			813	26.962				34.82
3551	CG			813	26.132	6.832	88.076		34.63
3552	CD1	TYR			25.269	7.812	88.444 89.559		29.08 29.89
3553		TYR			24.637	7.762			35.16
3554	CZ	TYR			24.749	6.694 6.732	90.445 91.691		33.13
3555	OH	TYR TYR			23.994	5.638	90.112		31.34
3556 3557	CE2 CD2				25.605 26.330	5.766			30.20
3557 3558	CD2	TYR TYR			29.301	6.978			34.15
3558	0			813	28.981		85.162		35.41
	N			814	30.513	7.539			33.63
3560	1.4	GLI	D	014	30.313	1.339	00.091	1.00	55.05

FIGURE 3BS

A	В	C	D	E	F	G	Н	I	J
3561	CA			814	31.485	6.912	85.013		33.04
3562	C			814	31.465	7.503	83.656		33.66
3563	0			814	31.929	6.919	82.671		29.15
3564	N			815	30.913	8.688	83.576		34.73
3565	CA			815	31.053	9.319	82.301		37.09
3566	CB			815	30.177	10.491	82.237		38.02
3567	CG			815	30.303	11.378	80.999		40.70
3568	CD			815	29.679	10.720	79.825		39.58
3569		GLU			30.404	10.091	79.087		37.45
3570		GLU			28.456	10.675	79.743		43.36
3571	C			815	32.498	9.735	82.095		38.19 38.65
3572 3573	O N			815 816	33.212 32.930	10.124 9.543	83.020 80.863		37.01
3573 3574	CA	ARG			34.213	9.930	80.391		38.78
3575	CB			816	34.213	9.446	78.966		38.98
3575 3576	CG	ARG			35.424	10.059	78.162		42.28
3577	CD	ARG			36.087	9.017	77.341		52.01
3578	NE	ARG			37.532	9.132	77.341	1.00	
3579	CZ	ARG			38.138	9.580	76.306	1.00	
3580		ARG			37.353	9.900	75.305	1.00	
3581		ARG			39.446	9.779	76.226	1.00	
3582	C	ARG			34.381	11.410	80.467		38.72
3583	0	ARG			33.687	12.139	79.791		39.78
3584	N			817	35.330	11.824	81.298		37.40
3585	CA			817	35.684	13.217	81.461		37.95
3586	CB			817	36.997	13.136	82.256		37.05
3587	CG			817	36.763	11.888	83.183		38.15
3588	CD	PRO	В	817	36.171	10.927	82.136	1.00	38.41
3589	С	PRO	В	817	35.788	13.947	80.089	1.00	38.69
3590	0	PRO	В	817	36.495	13.433	79.252	1.00	36.60
3591	N	TYR	В	818	35.057	15.066	79.844	1.00	38.82
3592	CA	TYR	В	818	35.210	15.759	78.539	1.00	39.23
3593	CB	TYR	В	818	36.663	16.068	78.236	1.00	38.09
3594	CG	TYR	В	818	37.266	16.821	79.315	1.00	39.70
3595	CD1	TYR			36.909	18.157	79.532	1.00	34.79
3596	CE1	TYR	В	818	37.443	18.905	80.645		34.86
3597	CZ	TYR	В	818	38.325	18.209	81.532		37.76
3598	OH	TYR	В	818	38.860				39.95
3599	CE2	TYR			38.653	16.824	81.335		33.51
3600	CD2	TYR			38.098	16.158	80.229		36.26
3601	C	TYR			34.667	14.938	77.424		38.80
3602	0	TYR			34.928	15.202	76.270		39.89
3603	N	TRP			33.846	13.989	77.763		38.70
3604	CA	TRP			33.188	13.270	76.700		39.85
3605	CB	TRP			32.069	14.135	76.151		38.03
3606	CG	TRP			31.456	14.694	77.287		36.05
3607	CD1	TRP			30.606	14.112	78.042		30.08
3608	NE1	TRP			30.225	14.945	79.039		25.80
3609	CE2	TRP			30.803	16.169	78.851		30.10
3610	CD2	TRP			31.604	16.053	77.781		36.77
3611	CE3	TRP			32.310	17.173	77.346		33.18
3612	CZ3	TRP	B	819	32.236	18.266	77.979	1.00	31.31

FIGURE 3BT

A	В	C	D	E	F		G		Н	I	J
3613	CH2	TRP	В	819	31.43	10	18.424	79.	081	1.00	35.76
3614	CZ2			819	30.6		17.374	79.	552	1.00	36.26
3615	C			819	34.1		12.981		636	1.00	39.50
3616	0	TRP	В	819	35.25	57	12.601	75.	950	1.00	42.24
3617	N	GLU	В	820	33.83	37	13.251	74.	389	1.00	39.99
3618	CA	GLU	В	820	34.74	42	12.918	73.	254	1.00	40.61
3619	CB	GLU	В	820	33.94	41	12.178	72.	114	1.00	41.25
3620	CG	GLU	В	820	33.26	63	10.859	72.	529	1.00	40.27
3621	CD	GLU	В	820	32.03	30	11.030	73.	446	1.00	45.99
3622	OE1	GLU	В	820	31.8	75	10.407	74.	529	1.00	48.82
3623	OE2	GLU	В	820	31.16	63	11.766	73.	086	1.00	36.20
3624	C	GLU	В	820	35.70	80	14.020	72.	749	1.00	40.02
3625	0	GLU	В	820	36.23	16	13.972	71.	706		39.30
3626	N	LEU	В	821	35.94	44	15.037	73.	516	1.00	42.32
3627	CA	LEU	В	821	36.96	69	16.002	73.	125	1.00	45.66
3628	CB	LEU	В	821	37.23	12	16.973		283		45.63
3629	CG	LEU	В	821	36.2	73	18.189	74.	253	1.00	
3630	CD1	LEU	В	821	34.84	48	17.908		740	1.00	
3631	CD2	LEU		821	36.25		18.988		530		46.51
3632	C	LEU		821	38.23		15.199		892		45.45
3633	0	LEU			38.30		14.137		411		45.58
3634	N			822	39.18		15.665		097		45.03
3635	CA			822	40.46		14.994		975		47.64
	CB			822	41.26		15.426		738	1.00	
3637	OG			822	41.44		16.836		727		44.19
3638	C	SER		822	41.29		15.448		115		48.61
3639	0	SER			40.9		16.431		769	1.00	
3640	N	ASN			42.40		14.776		341	1.00	
3641	CA	ASN			43.32		15.385		319	1.00	53.14
3642	CB	ASN			44.48		14.436		614	1.00	53.45
3643	CG	ASN			43.99		13.177		311	1.00	57.25 56.44
3644		ASN			42.9		13.236		090	1.00	
3645		ASN			44.64		12.035		027	1.00	50.82 52.98
3646	C	ASN			43.66		16.895 17.756		071 937	1.00	53.13
3647 3648	O N	ASN HIS		824	43.35 44.13		17.736		858	1.00	54.65
3649	CA	HIS			44.4		18.636		459	1.00	54.79
3650		HIS			45.03		18.740		973		58.59
3651	CG	HIS			44.12		19.419		940		67.70
3652		HIS			43.60		20.705		072		73.79
3653		HIS			42.88		21.017		000		
3654		HIS			42.76		20.940		073	1.00	
3655		HIS			42.93		19.999		157		76.47
3656		HIS			43.7		18.994		703		75.66
3657	C	HIS			43.30		19.509		778		52.56
3658	Ō	HIS			43.42		20.588		463		49.91
3659	N	GLU			42.12		19.027		387	1.00	
3660	CA	GLU			40.94		19.831		718	1.00	
3661	CB	GLU			39.69		19.255		086		52.70
3662	CG	GLU			39.95		18.712		695		55.19
3663	CD	GLU			38.70		18.188		065		60.55
3664		GLU			38.48	80	16.987		221		63.97

FIGURE 3BU

A	В	С	D	E	F	G	Н	I	J
3665	OE2	GLU	В	825	37.946	18.964	69.435	1.00	63.96
3666	С	GLU	В	825	40.747	20.079	74.206	1.00	49.70
3667	0	GLU	В	825	40.538	21.250	74.669	1.00	48.88
3668	N			826	40.903	19.012	74.976	1.00	47.68
3669	CA			826	40.825	19.160	76.439	1.00	46.21
3670	CB			826	41.173	17.756	77.124	1.00	47.64
3671		VAL			41.421	17.900	78.686	1.00	46.13
3672		VAL			40.130	16.592	76.663		38.86
3673	C			826	41.762	20.239	76.958		46.74
3674	Ō			826	41.363	21.236	77.651		46.61
3675	N			827	43.023	20.076	76.582		47.29
3676	CA			827	44.025	21.031	77.016	1.00	48.46
3677	CB			827	45.429	20.635	76.593		49.16
3678	CG			827	46.036	19.261	77.139		48.31
3679	SD			827	47.464	18.772	76.174	1.00	56.19
3680	CE			827	48.223	20.801	76.241	1.00	
3681	C			827	43.641	22.449	76.548	1.00	
3682	Ö			827	43.675	23.355	77.381	1.00	
3683	N			828	43.175	22.647	75.280	1.00	
3684	CA			828	42.812	23.992	74.874		48.64
3685	CB			828	42.467	24.087	73.404		49.40
3686	C			828	41.656	24.425	75.727		47.69
3687	0			828	41.688	25.516	76.302		45.93
3688	N			829	40.622	23.600	75.859	1.00	
3689	CA			829	39.500	24.095	76.706	1.00	
3690	CB			829	38.454	23.025	76.877	1.00	
3691	C			829	39.974	24.564	78.107	1.00	
3692	Ō			829	39.428	25.519	78.706	1.00	52.39
3693	N			830	40.902	23.804	78.674	1.00	51.92
3694	CA			830	41.427	24.108	79.998	1.00	
3695	CB			830	42.400	22.914	80.456	1.00	
3696	CG1			830	41.635	21.788	81.139	1.00	55.56
3697	CD1			830	40.775	22.243	82.301	1.00	
3698	CG2			830	43.521	23.378	81.390	1.00	52.02
3699	C			830	42.152	25.485	79.957	1.00	54.79
3700	0			830	41.872	26.417	80.751	1.00	54.16
3701	N	ASN	В	831	43.068	25.588	79.006	1.00	55.43
3702	CA	ASN			43.834	26.818	78.871	1.00	57.64
3703	CB	ASN			44.900	26.698	77.762	1.00	57.97
3704	CG			831	46.082	25.749	78.170	1.00	61.45
3705		ASN			46.313	25.407	79.388	1.00	63.42
3706	ND2	ASN	В	831	46.803	25.283	77.160	1.00	61.97
3707	C	ASN	В	831	42.869	28.013	78.776	1.00	56.48
3708	0	ASN	В	831	43.088	29.055	79.374	1.00	57.73
3709	N	ASP			41.729	27.833	78.136	1.00	55.50
3710	CA	ASP			40.747	28.879	78.162	1.00	54.22
3711	CB	ASP			39.824	28.726	76.982	1.00	56.03
3712	CG	ASP			40.475	29.240	75.659	1.00	62.62
3713	OD1	ASP	В	832	40.519	30.491	75.432	1.00	65.21
3714		ASP			41.001	28.469	74.822	1.00	63.16
3715	C	ASP	В	832	39.956	28.914	79.478	1.00	53.83
3716	0	ASP	В	832	39.026	29.722	79.634	1.00	49.78

FIGURE 3BV

37117 N GLY B 40.258 28.009 80.431 1.00 52.62 3718 C GLY B 333 39.487 28.103 81.674 1.00 52.59 3720 O GLY B 833 37.252 27.863 82.546 1.00 50.65 3721 N PHE B 34 37.755 26.621 80.730 1.00 49.17 3721 C PHE B 834 36.587 24.912 79.451 1.00 49.17 3723 CB PHE B 834 35.397 23.934 79.392 1.00 49.59 3725 CDI PHE B 34 35.538 22.592 79.676 1.00 48.43 3726 CEI PHE B 334 34.512 21.70 79.632 1.00 49.88 3727 CZ PHE B 334 31.10 23.31	A	В	С	D	E	F	G	Н	I	J
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37.19										
3720 O GLY B 833 37.252 27.863 82.546 1.00 53.45 3721 N PHE B 834 37.795 26.621 80.730 1.00 50.06 3722 CA PHE B 834 36.587 25.786 80.701 1.00 49.17 3723 CB PHE B 834 36.587 24.912 79.451 1.00 46.71 3724 CG PHE B 834 35.538 22.592 79.676 1.00 48.54 3725 CDI PHE B 834 35.538 22.592 79.676 1.00 48.54 3726 CEI PHE B 834 33.5538 22.592 79.676 1.00 49.59 3726 CDI PHE B 834 33.226 22.210 79.315 1.00 47.84 3728 CE2 PHE B 834 33.106 23.517 78.977 1.00 49.63 3728 CE2 PHE B 834 33.106 23.517 78.977 1.00 49.63 3730 C PHE B 834 33.106 23.517 78.979 1.00 49.93 3730 C PHE B 834 37.960 24.368 82.076 1.00 44.32 3733 CA ARG B 835 35.745 24.346 82.462 1.00 43.32 3733 CA ARG B 835 35.414 23.993 84.921 1.00 40.35 3734 CB ARG B 835 35.414 23.993 84.921 1.00 40.36 3735 CG ARG B 835 35.414 23.993 84.921 1.00 40.36 3736 CD ARG B 835 37.837 24.558 85.418 1.00 39.62 3736 CD ARG B 835 37.837 24.558 85.418 1.00 41.36 3739 NHI ARG B 835 39.981 25.049 86.127 1.00 43.02 3734 CB ARG B 835 39.981 25.049 86.127 1.00 44.32 3738 NHI ARG B 835 39.981 25.329 84.088 1.00 44.32 3734 CD ARG B 835 33.4440 22.546 83.165 1.00 44.62 3741 C ARG B 835 33.440 22.546 83.165 1.00 44.62 3741 C ARG B 835 33.440 22.546 83.165 1.00 40.49 3742 C ARG B 835 33.440 22.546 83.165 1.00 40.49 3742 C ARG B 836 33.425 20.396 83.233 1.00 37.66 3746 CG LEU B 836 33.425 20.396 83.233 1.00 37.66 3746 CG LEU B 836 33.425 20.396 83.233 1.00 37.63 3746 CG LEU B 836 33.425 20.396 83.233 1.00 37.63 3746 CG PRO B 837 29.824 21.275 84.187 1.00 34.92 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3753 CB PRO B 837 29.824 21.275 84.187 1.00 34.92 3753 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3753 CD PRO B 837 29.824 21.275 85.417 1.00 34.92 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.34 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3755 CD PRO B 837 29.824 21.275 84.187 1.00 34.92 3755 CD PRO B 837 29.824 21.275 85.511 1.00 3										
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FIGURE 3BW

A	В	C	D	E	F	. G	Н	I	J
3769	CD	PRO	В	839	28.056	17.580	88.467	1.00	42.30
3770	C			839	25.278	16.789	87.071	1.00	44.34
3771	0	PRO	В	839	24.955	17.610	87.915	1.00	46.72
3772	N	ALA	В	840	24.416	16.004	86.466	1.00	46.17
3773	CA	ALA	В	840	22.989	16.149	86.701	1.00	46.30
3774	CB	ALA	В	840	22.229	15.193	85.735	1.00	46.61
3775	C	ALA	В	840	22.791	15.690	88.100	1.00	47.32
3776	0	ALA	В	840	23.359	14.659	88.452	1.00	48.03
3777	N	ASP	В	841	21.963	16.400	88.859	1.00	47.66
3778	CA	ASP	В	841	21.685	16.142	90.292	1.00	48.16
3779	CB	ASP	В	841	20.927	14.837	90.420	1.00	50.16
3780	CG	ASP	В	841	19.492	14.998	89.877	1.00	56.15
3781	OD1	ASP	В	841	18.696	13.990	89.914	1.00	57.77
3782	OD2	ASP	В	841	19.120	16.143	89.372	1.00	56.22
3783	C	ASP	В	841	22.863	16.166	91.204	1.00	47.22
3784	0	ASP	В	841	22.887	15.601	92.244	1.00	48.47
3785	Ň	CYS	В	842	23.875	16.886	90.866	1.00	45.42
3786	CA	CYS	В	842	24.882	16.890	91.830		42.29
3787	CB	CYS		842	26.202	17.117	91.137		42.38
3788	SG	CYS		842	27.632	17.081	92.149		39.32
3789	C	CYS		842	24.617	17.957	92.802		43.32
3790	0	CYS			24.280	19.092	92.452		45.03
3791	N			843	24.714	17.602	94.064		43.72
3792	CA			843	24.628	18.589	95.111		42.14
3793	CB			843	24.991	17.794	96.325		44.83
3794	CG			843	24.594	16.246	95.888		42.62
3795	CD	PRO		843	24.689	16.198	94.536		40.73
3796	C	PRO		843	25.658	19.593	94.858		42.60
3797	0	PRO		843	26.804	19.223	94.460		43.32
3798	N	SER			25.288	20.847	95.134		40.74
3799	CA	SER			26.138	22.019	94.922		41.10
3800	CB	SER			25.378 24.007	23.281	95.359 95.667		45.78 47.77
3801	OG C	SER SER			27.363	22.921 22.044	95.753		39.64
3802	0	SER			28.384	22.625	95.733		40.26
3803 3804	N	ALA			27.313	21.508	96.965		37.83
3805	CA	ALA			28.582	21.420	97.650		36.40
3806	CB	ALA			28.347		99.043		39.16
3807	C	ALA			29.485	20.414	97.041		36.50
3808	0	ALA			30.717	20.568	96.981		40.92
3809	N			846	28.983	19.393	96.448		37.49
3810	CA	ILE			29.931	18.505	95.824		38.19
3811	CB	ILE			29.123	17.228	95.389		38.40
3812	CG1	ILE			28.802	16.375	96.633		41.00
3813	CD1	ILE			30.056	16.440	97.794		34.53
3814	CG2	ILE			29.935	16.381	94.424		38.32
3815	C	ILE			30.488	19.261	94.613		39.49
3816	0	ILE			31.719	19.363	94.292		37.89
3817	N	TYR			29.540	19.759	93.833		42.21
3818	CA	TYR			30.006	20.529	92.653		42.74
3819	CB	TYR			28.846	21.081	91.802		43.60
3820	CG	TYR			29.434	21.686	90.506		46.75

FIGURE 3BX

A	В	С	D	E	F	G	Н	I	J
2001	an 1	mvr.	_	0.47	20 220	22 225	00 140	1 00	40 15
3821	CD1			847	29.238	23.035	90.142		40.15 48.32
3822	CE1			847	29.804	23.528	88.926		46.32
3823	CZ			847	30.561 31.151	22.684 23.079	88.120 86.988		40.40
3824	OH CE2			847 847	30.776	23.079	88.509		44.70
3825 3826	CD2			847	30.776	20.893	89.685		47.08
3827	CD2			847	30.254	21.662	93.143		40.26
3828	0			847	31.963	21.877	92.659		40.34
3829	N			848	30.451	22.340	94.207		41.30
3830	CA			848	31.418	23.410	94.664		43.37
3831	CB			848	30.823	24.320	95.701		45.07
3832	CG			848	31.676	25.537	96.106	1.00	
3833	CD			848	31.283	26.899	95.372		63.54
3834	OE1			848	30.417	26.923	94.412		64.88
3835	NE2			848	31.976	28.042	95.806		60.42
3836	C			848	32.850	22.934	94.967		41.04
3837	0			848	33.897	23.527	94.527		41.33
3838	N			849	32.915	21.786	95.608		38.01
3839	CA	LEU	В	849	34.208	21.204	95.905	1.00	35.47
3840	CB	LEU	В	849	33.889	20.040	96.868	1.00	36.49
3841	CG			849	35.120	19.349	97.222	1.00	36.62
3842	CD1	LEU	В	849	36.078	20.393	97.866	1.00	32.52
3843	CD2	LEU	В	849	34.708	18.241	98.241	1.00	43.70
3844	C	LEU	В	849	34.946	20.716	94.708	1.00	35.06
3845	0	LEU	В	849	36.200	20.891	94.564	1.00	34.28
3846	N	MET	В	850	34.223	20.003	93.821	1.00	35.02
3847	CA	MET	В	850	34.861	19.681	92.512	1.00	36.09
3848	CB	MET	В	850	33.703	19.134	91.632		37.35
3849	CG	MET	В	850	33.905	18.476	90.380		32.97
3850	SD			850	32.372	17.871	89.923		36.02
3851	CE			850	31.755	17.245	91.136		32.09
3852	C			850	35.487	21.062	92.000		36.72
3853	0			850	36.645	21.219	91.693		
3854	N			851	34.747	22.126	91.975		37.60
3855	CA			851	35.408	23.296	91.429	1.00	
3856	CB	MET			34.424	24.425	91.381 90.395	1.00	
3857	CG	MET		851	33.322 33.760	24.168	88.645	1.00	45.90
3858	SD		_				88.676		46.07
3859	CE			851	34.669 36.688				41.53
3860 3861	С О	MET		851 851	37.765	24.106			43.20
	N	GLN			36,617		93.495		38.35
3862 3863	CA			852	37.772	24.172	94.206		39.33
3864	CB			852	37.474	24.172	95.703		42.34
3865	CG			852	36.356	25.195	96.036		45.28
3866	CD			852	35.754	24.863	97.391		62.60
3867		GLN			34.797	25.545			68.59
3868		GLN			36.292	23.806			69.44
3869	C			852	38.834	23.236	93.879		40.26
3870	0			852	39.939	23.631	93.706		41.90
3871	N			853	38.590				40.71
3872	CA			853	39.835	21.254	93.263		39.23

FIGURE 3BY

A	В	C	D	E		F	G		Н	I	J
3873	СВ	CYS	В	853	39.	. 782	19.71	1 93	3.273	1.00	39.20
3874	SG	CYS	В	853	38.	.918	18.95		1.690	1.00	40.47
3875	С	CYS	В	853	40.	.318	21.68		1.913	1.00	40.72
3876	0	CYS	В	853	41.	.421	21.34	7 9:	1.564	1.00	38.66
3877	N	TRP	В	854	39.	.519	22.36	6 93	1.092	1.00	41.68
3878	CA	TRP	В	854	40.	.111	22.64	7 89	9.772	1.00	44.18
3879	CB	TRP	В	854	39.	.031	22.45	7 88	3.667	1.00	44.45
3880	CG	TRP	В	854	38.	618	21.11	4 88	3.501		41.82
3881	CD1	TRP	В	854	39.	.368	19.98	0 88	3.704		41.87
3882	NE1			854		.602	18.86		3.449		35.93
3883	CE2			854		. 352	19.26		3.140		32.47
3884	CD2			854		. 333	20.68		3.167		38.06
3885	CE3			854		.138	21.35		7.897		32.76
3886	CZ3			854		.127	20.66		7.536		29.91
3887	CH2			854		.159	19.21		7.528		36.45
3888	CZ2			854		.282	18.52		7.789		32.15
3889	C			854		.722	24.08		9.583		45.26
3890	0	TRP		854		.080	24.49		3.441		43.51
3891	N	GLN		855		.727	24.84		0.675		45.68
3892	CA	GLN		855		.226	26.18		0.651		46.55
3893	CB			855		.379	26.72		2.049		48.28 50.56
3894	CG CD			855 855		.053 .145	26.99 28.20		2.625 3.423		60.72
3895	OE1	GLN GLN		855		.024	28.13		1.670		58.07
3896 3897	NE2			855		. 408	29.38		2.729		61.21
3898	C			855		.519	26.13		0.037		45.75
3899	0			855		.278	25.30		0.342		42.80
3900	N			856		710	27.05		9.106		47.78
3901	CA			856		924	27.24		3.368		47.38
3902	СВ			856		729	28.48		7.470		49.87
3903	CG			856		.834	28.69		5.488		49.20
3904	CD	GLN		856		.839	27.59		5.453		59.89
3905	OE1	GLN	В	856	43.	.788	26.94	7 85	5.185	1.00	61.37
3906	NE2	GLN	В	856	46.	.017	27.35	6 84	1.866	1.00	60.84
3907	C	GLN	В	856	45.	.065	27.45	6 89	9.331	1.00	46.71
3908	0	GLN	В	856	46.	.106	26.88	3 89	9.154		44.54
3909	N	GLU		857	44.	.892	28.30		0.331		48.11
3910	CA	GLU	В	857			28.40	8 93	1.341	1.00	51.65
3911	CB	GLU	В	857		.768	29.57		2.387		52.14
3912	CG			857		.166	30.91		1.710		62.33
3913	CD			857		.832	32.25		2.398		71.26
3914		GLU				616	32.36		3.641		76.69
3915		GLU				.828	33.23		L.631		75.04
3916	C			857		.160	27.13		2.117		49.78
3917	0			857		368	26.87		3.003		50.77
3918	N	ARG				.167	26.34		1.823		48.84
3919	CA			858		.332	25.17		2.679		48.89
3920	CB	ARG				631	24.42		2.402		48.75
3921	CG			858		933	24.99		2.988		46.77 55.09
3922	CD			858		166	24.44		2.169 2.946		66.77
3923	NE CZ			858		374	24.18		2.946		70.86
3924	CZ	AKG	B	858	53.	.580	24.70	0 92	2./06	1.00	70.00

FIGURE 3BZ

A	В	C	D	E	F	G	Н	I	J
3925	NH1	ARG	В	858	53.804	25.519	91.672	1.00	68.19
3926		ARG			54.588	24.373	93.510		75.23
3927	C			858	47.192	25.455	94.211		49.58
3928	0	ARG		858	46.606	24.640	94.922		47.02
3929	N	ALA		859	47.743	26.584	94.704		49.56
3930	CA	ALA			47.766	26.775	96.131		49.75
3931	CB			859	48.584	27.954	96.533		51.56
3932	C			859	46.364	26.871	96.691		49.92
3933	Ō			859	46.123	26.666	97.946		47.88
3934	N			860	45.410	27.081	95.789		47.89
3935	CA			860	44.084	27.368	96.360		46.93
3936	СВ			860	43.377	28.492	95.576		48.07
3937	C			860	43.240	26.131	96.356		45.49
3938	0			860	42.064	26.182	96.738		43.79
3939	N			861	43.808	25.041	95.824		45.18
3940	CA			861	43.069	23.742	95.850		45.03
3941	CB			861	43.616	22.678	94.889	1.00	45.11
3942	CG			861	43.572	23.172	93.351		46.90
3943	CD	ARG		861	44.345	22.261	92.433		44.77
3944	NE			861	44.743	22.970	91.264	1.00	
3945	CZ			861	45.809	22.714	90.575	1.00	
3946		ARG			46.592	21.700	90.905	1.00	
3947	NH2	ARG			46.150	23.523	89.537	1.00	43.27
3948	С	ARG	В	861	43.130	23.309	97.271	1.00	45.07
3949	0	ARG			44.103	23.626	98.032	1.00	44.45
3950	N	PRO	В	862	42.026	22.694	97.660	1.00	43.87
3951	CA	PRO	В	862	41.895	22.193	98.984	1:00	43.84
3952	CB	PRO	В	862	40.554	21.463	98.980	1.00	44.25
3953	CG	PRO	В	862	39.896	21.841	97.717	1.00	41.03
3954	CD	PRO	В	862	40.829	22.473	96.845	1.00	44.03
3955	C	PRO	В	862	42.931	21.188	99.086	1.00	43.12
3956	0	PRO	В	862	43.244	20.570	98.142	1.00	42.37
3957	N	LYS	В	863	43.431	21.006	100.274	1.00	43.78
3958	CA	LYS	В	863	44.308	19.872	100.517	1.00	44.01
3959	CB	LYS	В	863	45.168	20.223	101.764		44.71
3960	CG	LYS			46.523	20.788	101.339		51.54
3961	CD	LYS			46.460	22.176	100.652		56.44
3962	CE	LYS			47.864		100.246		61.29
3963	NZ	LYS			49.033		100.373		67.02
3964	C			863	43.545		100.706		39.71
3965	0			863	42.327		101.170		38.33
3966	N			864	44.230		100.460		36.76
3967	CA			864	43.420		100.759		38.90
3968	CB			864	44.140		100.429		37.94
3969	CG			864	44.178	14.527			33.91
3970		PHE			45.375	14.533	98.233		29.69
3971		PHE			45.459	14.319			34.24
3972	CZ			864	44.247	14.052			34.64
3973		PHE			43.040	14.039			34.40
3974	CD2				43.011				33.00
3975	C			864	42.796		102.134		39.31
3976	0	rnE	В	864	41.644	T2.0T0	102.340	Ι.ΟΟ	42.22

FIGURE 3CA

A	В	C	D	E	F	G	H	I	J
3977	N	ALA	В	865	43.535	16.632	103.081	1.00	38.65
3978	CA	ALA	В	865	43.021		104.387	1.00	41.81
3979				865	44.179	16.905	105.512	1.00	42.20
3980	C			865	41.864	17.534	104.488	1.00	41.60
3981	0			865	40.936		105.218		41.67
3982	N			866	41.882	18.696	103.846		42.39
3983	CA			866	40.590	19.411	104.022		44.31
3984	CB			866	40.540	20.833	103.439		44.90
3985	CG			866	41.770		103.675		50.05
3986		ASP			42.078		104.884		55.78
3987		ASP			42.487		102.707		49.26
3988	C			866	39.398		103.357	1.00	
3989	0			866	38.289		103.908		40.88
3990	N	ILE		867	39.687	17.950	102.214		41.48
3991	CA			867	38.644		101.454		39.52
3992	CB			867	39.235		100.175	1.00	39.26
3993	CG1			867	39.557	17.782	99.199		37.38
3994	CD1			867	40.457	17.388	97.911	1.00	34.65
3995	CG2			867	38.265	15.618	99.527	1.00	30.26
3996	C			867	38.010	16.203	102.272	1.00	39.36
3997	0			867	36.787		102.304		37.24
3998	N	VAL		868	38.841	15.458	102.980		40.82
3999	CA			868	38.200		103.809		40.27
4000	CB	VAL		868	39.269		104.586		43.83
4001	CG1			868	38.560		105.520		38.82
4002	CG2	VAL			40.125		103.646		39.45
4003	C			868	37.345		104.808		40.69
4004	O N			868	36.193	14.723	105.003		41.29
4005	N CA			869 869	37.826	16.169			41.17
4006	CB			869	36.879	16.666	106.516		44.54
4007 4008	OG			869	37.479	17.651 18.378	107.541 106.941		46.64 50.61
4008	C			869	38.536		105.941		44.10
4009	0			869	35.713 34.559	17.140	105.912		45.09
4010	N			870	35.941	17.140	100.449		43.54
4012	CA			870	34.744	18.495	104.771		42.08
4013	CB			870	34.755	19.950	103.300		43.22
4014	CG1	ILE			33.586		102.312		41.61
4015	CD1			870	33.949		101.176		41.32
4016	CG2			870	36.033		102.635		40.07
4017	C			870	33.864		103.682		41.89
4018	0			870	32.658		103.793		41.51
4019	N	LEU			34.404	16.281	103.792		42.27
4020	CA	LEU			33.374	15.249	102.861		42.82
4021	CB	LEU			33.923	14.113	101.973		40.18
4022	CG	LEU			34.172	14.656	100.580		43.50
4023	CD1	LEU			34.974		99.846		42.97
4024	CD2	LEU			32.952		99.820		30.76
4025	C	LEU			32.699		104.115		41.38
4026	0	LEU			31.528		104.128		43.91
4027	N	ASP			33.394		105.207		41.15
4028	CA	ASP			32.653		106.384		41.49
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FIGURE 3CB

A	В	С	D	E	F	G	Н	I	J
4029	СВ	ASP	В	872	33.673	13.713	107.437	1.00	39.80
4030	CG	ASP			34.462	12.401	107.107	1.00	45.40
4031	OD1		В		33.894	11.494	106.424	1.00	51.78
4032		ASP			35.617	12.127		1.00	
4033	C	ASP			31.402	14.875	106.910		43.24
4034	0	ASP		872	30.268	14.269	107.347		42.17
4035	N	LYS		873	31.557	16.226	106.813	1.00	42.48
4036	CA	LYS	В		30.499	17.147	107.252	1.00	45.45
4037	СВ			873	30.925	18.620	107.369	1.00	46.52
4038	ĊĠ	LYS	В	873	32.038	18.846	108.362	1.00	52.07
4039	CD	LYS	В	873	32.946	20.036	107.986	1.00	60.03
4040	CE	LYS	В	873	33.740	20.457	109.190	1.00	66.29
4041	NZ	LYS	В	873	34.221	19.164	109.838	1.00	72.68
4042	C	LYS	В	873	29.324	17.049	106.377	1.00	47.08
4043	0	LYS	В	873	28.196	17.131	106.833	1.00	48.85
4044	N	LEU	В	874	29.503	16.815	105.094	1.00	46.56
4045	CA	LEU	В	874	28.235	16.640	104.425	1.00	45.19
4046	CB	LEU	В	874	28.375	16.817	102.875		46.34
4047	CG	LEU	В	874	29.232	18.022	102.434	1.00	48.30
4048	CD1	LEU	В	874	29.940	17.832	101.164	1.00	45.32
4049	CD2	LEU	В	874	28.475	19.386	102.439	1.00	51.85
4050	C	LEU	В	874	27.677	15.295	104.767		46.11
4051	0	LEU	В	874	26.433	15.095	104.797		42.90
4052	N			875	28.568		104.846		48.45
4053	CA			875	28.076	12.933	105.024		49.62
4054	CB			875	29.276	11.927	105.013		50.00
4055	CG1			875	29.557	11.427	103.630		49.38
4056	CD1			875	30.973	10.853	103.455	1.00	50.85
4057	CG2			875	29.010	10.708	105.957	1.00	
4058	C			875	27.452	13.055		1.00	52.40
4059	0			875	26.435	12.478	106.683	1.00	
4060	N	ARG			28.026	13.876	107.267		55.97
4061	CA	ARG		876	27.371	13.957			59.43
4062	CB			876	28.395	14.347	109.636		60.00
4063	CG			876	28.796		110.592		61.19
4064	CD	ARG		876	29.309		110.037		67.05
4065	NE			876	30.770	11.823	110.044	1.00	76.99
4066	CZ			876	31.568		111.116		79.95
4067		ARG			32.887		110.939 112.335		81.01 79.88
4068		ARG			31.067				61.31
4069	C			876	26.149		108.667		63.40
4070	O N			876	25.336		109.576 107.728		61.95
4071	N			877	25.990		107.728		60.39
4072	CA	ALA			24.782		107.724		61.56
4073	CB C	ALA			25.142		106.099		60.30
4074 4075	0	ALA ALA			24.104 24.050		105.548		59.22
4075	N			878	23.522		105.546		60.43
4075	CA			878	23.006		104.833		60.43
4077	CB			878	22.159		104.833		60.78
4079	CG			878.	22.139		105.162		59.55
4079	CD			878	23.223		100.336		61.36
4000	CD	PRU	Б	0/0	43.443	14.400	107.139	1.00	01.30

FIGURE 3CC

A	В	С	D	E	F	G .	Н	I	J
4081	C	PRO	В	878	22.093	16.025	104.243	1.00	60.68
4082	Ö			878	21.843	15.907			60.12
4083	N	ASP		879	21.492	16.871			59.38
4084	CA			879	20.644	17.925			59.16
4085	CB			879	19.959	18.741			59.04
4086	CG			879	18.427	18.579			66.19
4087	OD1			879	17.726	19.586			72.48
4088	OD2			879	17.829	17.463		1.00	
4089	C			879	21.462	18.826	103.603	1.00	57.43
4090	0			879	20.981	19.301	102.590	1.00	57.64
4091	N			880	22.716	19.032	103.975	1.00	56.33
4092	CA	SER	В	880	23.644	19.836	103.267	1.00	54.79
4093	CB	SER	В	880	24.929	19.797	104.005	1.00	55.24
4094	OG	SER	В	880	25.622	18.605	103.690	1.00	55.50
4095	C	SER	В	880	23.879	19.301	101.868	1.00	54.99
4096	0	SER	В	880	24.507	19.979	101.077		53.72
4097	N	LEU	В	881	23.348	18.113	101.566	1.00	55.55
4098	CA	LEU	В	881	23.478	17.516	100.243	1.00	56.64
4099	CB	LEU	В	881	23.957	16.066		1.00	55.16
4100	CG	LEU	В	881	25.385	16.073			47.41
4101	CD1	LEU			25.879	14.711			44.25
4102	CD2	LEU			26.234	16.645	99.827		38.61
4103	С			881	22.260	17.570	99.338		60.26
4104	0	LEU			22.311	17.141	98.189		61.01
4105	N	ALA			21.141	18.068	99.839		64.54
4106	CA	ALA			19.923	18.077			66.81
4107	CB	ALA			18.619	18.004			66.76
4108	C	ALA			19.875	19.245			68.16
4109	0	ALA			19.531	19.064	96.866		69.24
4110	N	ALA			20.126	20.446	98.515		68.60
4111	CA	ALA			20.325	21.591 22.901	97.630 98.461		69.28 69.49
4112 4113	CB C	ALA ALA			20.372 21.685	21.361	96.886		69.14
4113	0	ALA			21.818	21.501	95.652		68.44
4114		ATP			46.712	-3.440			89.49
4147	PA	ATP			45.850	-2.328			84.33
4148		ATP			45.971	-1.113	87.512		78.95
4149		ATP					84.993		
4150	PB				47.730		84.575		98.93
4151		ATP			48.070		83.230		99.05
4152		ATP			48.948		85.490		95.56
4153		ATP			47.340		84.490		
4154	PG	ATP				0.614			101.51
4155		ATP			45.916			1.00	97.15
4156		ATP				0.728			95.81
4157		ATP			44.985	-0.323			99.53
4158		ATP			44.345	-2.779			81.43
4159		ATP			44.056	-3.806			76.05
4160	C4*	ATP	В1	L001	42.586	-4.122	85.531	1.00	72.65
4161	04*	ATP	BI	1001	42.294	-5.396	86.149		66.71
4162		ATP			41.362	-5.132	87.170	1.00	60.60
4163	C2*	ATP	B1	L001	40.769	-3.740	86.836	1.00	62.85

FIGURE 3CD

A	В	С	D	E	F	G	H	I	J
								*	
4164	02*	ATP	В1	001	40.111	-3.694	85.57	6 1.00	60.83
4165	C3*	ATP	В1	001	42.005	-3.004	86.42	4 1.00	67.86
4166	03*	ATP	В1	001	41.724	-1.884	85.61	2 1.00	68.16
4167	N9	ATP	В1	001	42.167	-5.202	88.43	4 1.00	53.63
4168	C8	ATP	В1	001	43.500	-4.813	88.65	5 1.00	53.17
4169	N7	ATP	В1	001	43.833	-5.108	89.97	0 1.00	50.95
4170	C5	ATP	В1	001	42.701	-5.612	90.61	9 1.00	46.80
4171	C6	ATP	В1	001	42.436	-6.005	91.94	9 1.00	44.40
4172	N6	ATP	B1	001	43.185	-5.600	93.06	7 1.00	37.97
4173	C4	ATP	B1	001	41.684	-5.687	89.65	2 1.00	48.42
4174	N3	ATP	B1	001	40.432	-6.108	89.96	5 1.00	44.97
4175	C2	ATP	В1	001	40.181	-6.529	91.25	3 1.00	46.46
4176	N1	ATP	В1	001	41.180	-6.522	92.17	9 1.00	41.31